

AD-775 373

CALCULATED ABSORPTION COEFFICIENTS FOR  
DF LASER FREQUENCIES

R. K. Long, et al

Ohio State University

Prepared for:

Advanced Research Projects Agency

November 1973

DISTRIBUTED BY:

**NTIS**

National Technical Information Service  
U. S. DEPARTMENT OF COMMERCE  
5285 Port Royal Road, Springfield Va. 22151

AD-775 373

CALCULATED ABSORPTION COEFFICIENTS FOR  
DF LASER FREQUENCIES

R. K. Long, et al

Ohio State University

Prepared for:

Advanced Research Projects Agency

November 1973

DISTRIBUTED BY:

**NTIS**

National Technical Information Service  
U. S. DEPARTMENT OF COMMERCE  
5285 Port Royal Road, Springfield Va. 22151

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER  RADC-TR-73-389	2. GOVT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) Calculated Absorption Coefficients for DF Laser Frequencies		5. TYPE OF REPORT & PERIOD COVERED  Interim
7. AUTHOR(s) R. K. Long F. S. Mills G. L. Trusty		6. PERFORMING ORG. REPORT NUMBER 3271-7
9. PERFORMING ORGANIZATION NAME AND ADDRESS The Ohio State Univ. Electroscience Lab Dept of Elec Engineering Columbus, OH 43212		8. CONTRACT OR GRANT NUMBER(s)  F30602-72-C-0016
11. CONTROLLING OFFICE NAME AND ADDRESS Advanced Research Projects Agency 1400 Wilson Blvd Arlington, VA 22209		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS PEC 62301E Proj 1279 Task 05
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office) Rome Air Development Center Griffiss AFB NY 13441		12. REPORT DATE Nov 1973
		13. NUMBER OF PAGES 78
		15. SECURITY CLASS. (of this report)  UNCLASSIFIED
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE
16. DISTRIBUTION STATEMENT (of this Report) Approved for public release; distribution unlimited		
17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)  Same as above		
18. SUPPLEMENTARY NOTES Monitored by: James W. Cusack, RADC/OCSE Griffiss AFB NY 13441		
19. KEY WORDS (Continue on reverse side if necessary and identify by block number) DF Laser                      Infrared Absorption                      Nitrogen Laser Propagation              Atmospheric Transmittance Water Vapor                      Methane Molecular Absorption              Nitrous Oxide		
20. ABSTRACT (Continue on reverse side if necessary and identify by block number) This report presents calculations of DF laser absorption coefficients for the Mid-Latitude Summer sea level atmospheric model. The individual gases which cause the absorption at each laser wavelength are identified. Results are compared with those previously published by R. A. McClatchey. The calculated results are being used to guide the experimental measurement program.		

DD FORM 1473  
1 JAN 73

EDITION OF 1 NOV 65 IS OBSOLETE

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

CALCULATED ABSORPTION COEFFICIENTS FOR  
OF LASER FREQUENCIES

R. K. Long  
F. S. Mills  
G. L. Trusty

Contractor: The Ohio State University  
Contract Number: F30602-72-C-0016  
Effective Date of Contract: 23 June 1971  
Contract Expiration Date: 31 March 1973  
Amount of Contract: \$130,000.00  
Program Code Number: OE20

Principal Investigator: Dr. Ronald K. Long  
Phone: 614 422-6077

Contract Engineer: James W. Cusack  
Phone: 315 330-3145

Approved for public release;  
distribution unlimited.

This research was supported by the  
Defense Advanced Research Projects  
Agency of the Department of Defense  
and was monitored by James W. Cusack,  
RADC (OCSE), GAFB, NY 13441 under  
contract F30602-72-C-0016.

## FOREWORD

This report, Ohio State University Research Foundation Report Number 3271-7 (seventh Quarterly Report), was prepared by the Ohio State University ElectroScience Laboratory, Department of Electrical Engineering at Columbus, Ohio. Research was conducted under Contract F30602-72-C-0016. Mr. James W. Cusack, RADC (OCSE), of Rome Air Development Center, Griffiss Air Force Base, New York, is the Project Engineer.

## PUBLICATION REVIEW

This technical report has been reviewed and is approved.

  
RADC Project Engineer

## ABSTRACT

This report presents calculations of DF laser absorption coefficients for the Mid-Latitude Summer sea level atmospheric model. The individual gases which cause the absorption at each laser wavelength are identified. Results are compared with those previously published by R. A. McClatchey. The calculated results are being used to guide the experimental measurement program.

## TABLE OF CONTENTS

	Page
I. INTRODUCTION	1
II. DETAILS OF THE DF CALCULATIONS	1
III. COMPUTED MID-LATITUDE SUMMER ABSORPTION COEFFICIENTS	5
IV. PLOTS	10
V. COMPARISON TO AFCRL CALCULATIONS	11
APPENDIX A	68
REFERENCES	72



## I. INTRODUCTION

The best information, prior to experiments, as to the expected molecular absorption coefficients at DF laser wavelengths are obtainable from calculations based upon the Air Force Cambridge Research Laboratories line data tape[1]. Dr. R. A. McClatchey has published a report containing DF predictions based on the data tape[2]. The calculations presented here are extensions of that work in that:

- 1) The list of laser lines is different. Our line list includes all of the lines which have been observed in our pulsed probe laser, some of which were not included in the McClatchey report. Also we now have new wavenumbers for some of the lines.
- 2) A small correction for the H<sub>2</sub>O continuum absorption which was omitted by McClatchey has been included. The data for this continuum absorption is given in the report on the AFCRL line data[1] which in turn is based on experimental work done by Burch[3].
- 3) Our calculations are presented only for one of McClatchey's atmospheric models (Mid-Latitude Summer) and only for sea level. We have, however, given the absorption coefficients for each component gas as well as the total coefficient so that one can see the relative importance of each absorber at each wavelength.
- 4) We have also made plots for each absorbing gas. These plots generally cover 5 or 10 wavenumbers to a page so that the laser line position relative to the absorption lines can be clearly seen. This is helpful in deciding whether small errors in either the absorption or laser line positions could result in a large change in the predicted coefficient.
- 5) Finally a calculation was made using a super-Lorentz line shape for the water vapor[4] in order to see what effect this would have on the coefficients.

## II. DETAILS OF THE DF CALCULATIONS

All of the calculations were made for the AFCRL[5] mid-latitude sea level summer model. Table I lists some of the pertinent data. The derivation of the various conversion factors used is given in Appendix A.



TABLE I  
Source of Absorption Line Data: AFCRL/GOAT TAPE  
Atmospheric Model: AFCRL Mid-Latitude Summer

---

T	= 294 °K
P	= 760 torr
p(H <sub>2</sub> O)	= 14.26 torr
p(N <sub>2</sub> O)	= 2.13E-4 (.28 ppm)
p(CH <sub>4</sub> )	= 1.216E-3 torr (1.6 ppm)
p(CO <sub>2</sub> )	= .251 torr (330 ppm)
p(O <sub>3</sub> )	= 2.31E-5 torr (6E-5 g/m <sup>3</sup> )
p(CO)	= 5.70E-5 torr (.075 ppm)

---

N<sub>2</sub> Continuum: AFCRL Report 434, Fig. 4.[1]

H<sub>2</sub>O Continuum: AFCRL Report 434, Fig. 2.[1]

Bound = 25 cm<sup>-1</sup>

---

The calculated absorption coefficients consist of three components: (1) molecular absorption, (2) water vapor continuum, and (3) pressure induced nitrogen absorption.

The data for the molecular absorption component was calculated using the AFCRL data tape[1]. This tape contains values for the frequency, strength, half-width, and lower energy state for H<sub>2</sub>O, N<sub>2</sub>O, CH<sub>4</sub>, CO<sub>2</sub>, CO, O<sub>3</sub>, and O<sub>2</sub> lines in the wavelength band of interest. In our calculations a Lorentz line shape was used with all lines within 25 cm<sup>-1</sup> of the calculation frequency being included in the summation. Another program parameter (SLOW) allows the exclusion of lines having a line strength less than SLOW from the summation if desired in order to save computer time. For this report SLOW was set to 10<sup>-27</sup> to effectively include all lines in the data tabulation.

The program computes  $\ln T = -k u$  where T is the fractional transmittance, k is the absorption coefficient in (mol-cm<sup>-2</sup>)<sup>-1</sup> and u is the absorber amount in mol-cm<sup>-2</sup>.

The line strength is defined as  $S = \int k dv$  and is in units of cm<sup>-1</sup>(mol-cm<sup>-2</sup>)<sup>-1</sup>. The halfwidth is in cm<sup>-1</sup>. The Lorentz shape is given by

$$(1) \quad k = \sum_i \frac{S_i \alpha_i}{\pi[(\nu - \nu_i)^2 + \alpha_i^2]}$$

The line strengths and half-widths are given at STP and must be corrected to model conditions. We have used the following relationships.

1. Halfwidth

$$(2) \quad \alpha_i = \alpha_{i0} \left( \frac{P_e}{P_0} \right) \left( \frac{T_0}{T} \right)^{CX}$$

The effective pressure  $P_e$  [8] is given by

$$(3) \quad P_e = \frac{B P_a + F P_f}{760} \text{ atmospheres}$$

where

$P_a$  = absorber pressure in torr

$P_f$  = broadener pressure in torr

$B$  = self-broadening coefficient

$F$  = foreign-broadening coefficient.

For nitrogen  $F$  is equal to one and the empirical values for  $B$ , assuming nitrogen broadening, are given in Table II for each gas [8].

TABLE II

	B	BX	CX
N <sub>2</sub> O	1.24	1.0	.5
CH <sub>4</sub>	1.3	1.5	.5
H <sub>2</sub> O	5.	1.5	.62
CO <sub>2</sub>	1.3	1.0	.58
O <sub>3</sub>	1.0	1.5	.5
CO	1.02	1.0	.5

The exponent CX is also given in Table II. Although theoretically CX = 0.5 for all of the gases, we have used for H<sub>2</sub>O and CO<sub>2</sub> the average empirical values originally suggested by Calfee and Benedict[9].

The line strengths were corrected to the model temperature by use of the relation

$$(4) \quad S_i = S_{i0} \left( \frac{T_0}{T} \right)^{BX} \exp \left( \frac{-E''}{k} \frac{T_0 - T}{T_0} \right)$$

where  $k = 0.6951 \text{ cm}^{-1}/\text{deg K}$   
 $E'' = \text{lower energy state in cm}^{-1} \text{ from data tape.}$

The coefficients BX for each of the molecules are listed in Table II.

The absorber amount, u, was computed from the formula

$$(5) \quad u = .733952 \times 10^{22} (p_a/760/T) \cdot \lambda \text{ mol-cm}^{-2}$$

where  $p_a = \text{absorber partial pressure in torr} = \text{ppm by volume} \times 10^{-6} \times P$   
 $T = \text{model temperature in deg K}$   
 $\lambda = \text{path in cm.}$   
 $P = \text{total pressure in torr.}$

Our program accepts the absorber partial pressure  $p_a$  in torr with the values given in Table I being used for the present work.

The AFCRL mid-latitude summer model gives the sea level H<sub>2</sub>O density as 14.1 gm/m<sup>3</sup> and using Eq. (3) of Appendix A the resulting  $p_a$  is 14.26 torr.

It is useful to note that there are 2438 water lines tabulated on the data tape between 2400 and 2850 cm<sup>-1</sup> of which 2150 or 88% are HDO. Also a composition factor of 0.03% for the HDO was assumed in compilation of the tape[1]. It is noted that this composition differs from the value of 0.027% which was given in the earlier water vapor data compilation by Gates, Calfee, Hansen and Benedict.

It is necessary in connection with the computation of absorber amount to have conversion factors between various systems of units. Although this information is available elsewhere[5,10] the derivations and resulting constants have been given in Appendix A of this report.

The water vapor continuum and pressure induced nitrogen absorption coefficients were derived from Figs. 2 and 4, respectively, of Reference [1].

Figure i which was derived from the experimental data of Burch[3] shows the wavelength dependence of the water vapor continuum absorption coefficient for 14.26 torr water vapor at sea level. The sea level absorption coefficient for 296°K and 14.26 torr H<sub>2</sub>O is given by

$$k(\nu) = 1.813 \times 10^{25} p_a^2 C_s^0(\nu) \text{ km}^{-1}$$

where  $C_s^0$  is from Burch's data and  $P_a$  is the H<sub>2</sub>O pressure in atmospheres.

Note that Burch[3] measured a  $C_s/C_b$  of approximately 8 whereas a value of 5 was assumed in the line by line calculations, see Table II. Also note that the Burch results used here (296°K) are actually extrapolated from measurements made at higher temperatures[3].

Figure ii shows the nitrogen absorption coefficient at 296°K[1]. The calculations in this report are all for a pressure of one atmosphere, thus the values from Fig. ii are used directly.

### III. COMPUTED MID-LATITUDE SUMMER ABSORPTION COEFFICIENTS

The calculated results for 30 DF laser lines are given in Table III. The six components which make up the total absorption coefficient are tabulated separately.

The AFCRL data tape lists no CO lines between 2400 and 2850 cm<sup>-1</sup> and the ozone absorption coefficient at the 30 DF lines was less than 10<sup>-5</sup> km<sup>-1</sup> for a concentration of 6 x 10<sup>-5</sup> g/m<sup>3</sup>. Therefore these two gases are not included.

Except for six DF lines between 2546.42 and 2594.25 cm<sup>-1</sup>, nearly all of the absorption is caused by water vapor and nitrogen. For these six lines N<sub>2</sub>O absorption is a significant factor. In the concentrations assumed, CH<sub>4</sub> absorption is a minor factor for all lines.

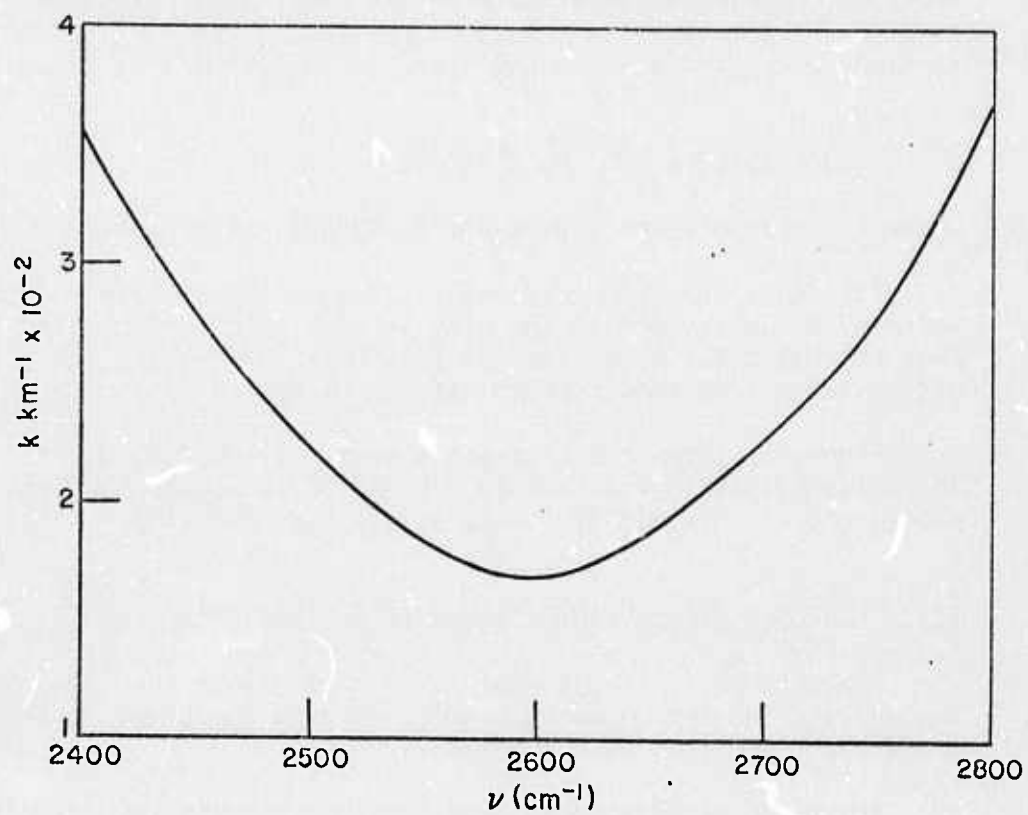


Fig. i. Water vapor continuum absorption coefficient adapted from Burch #4784[3] for  $p_{\text{H}_2\text{O}} = 14.2$  torr and  $T = 296^\circ\text{K}$  at 760 torr total pressure.

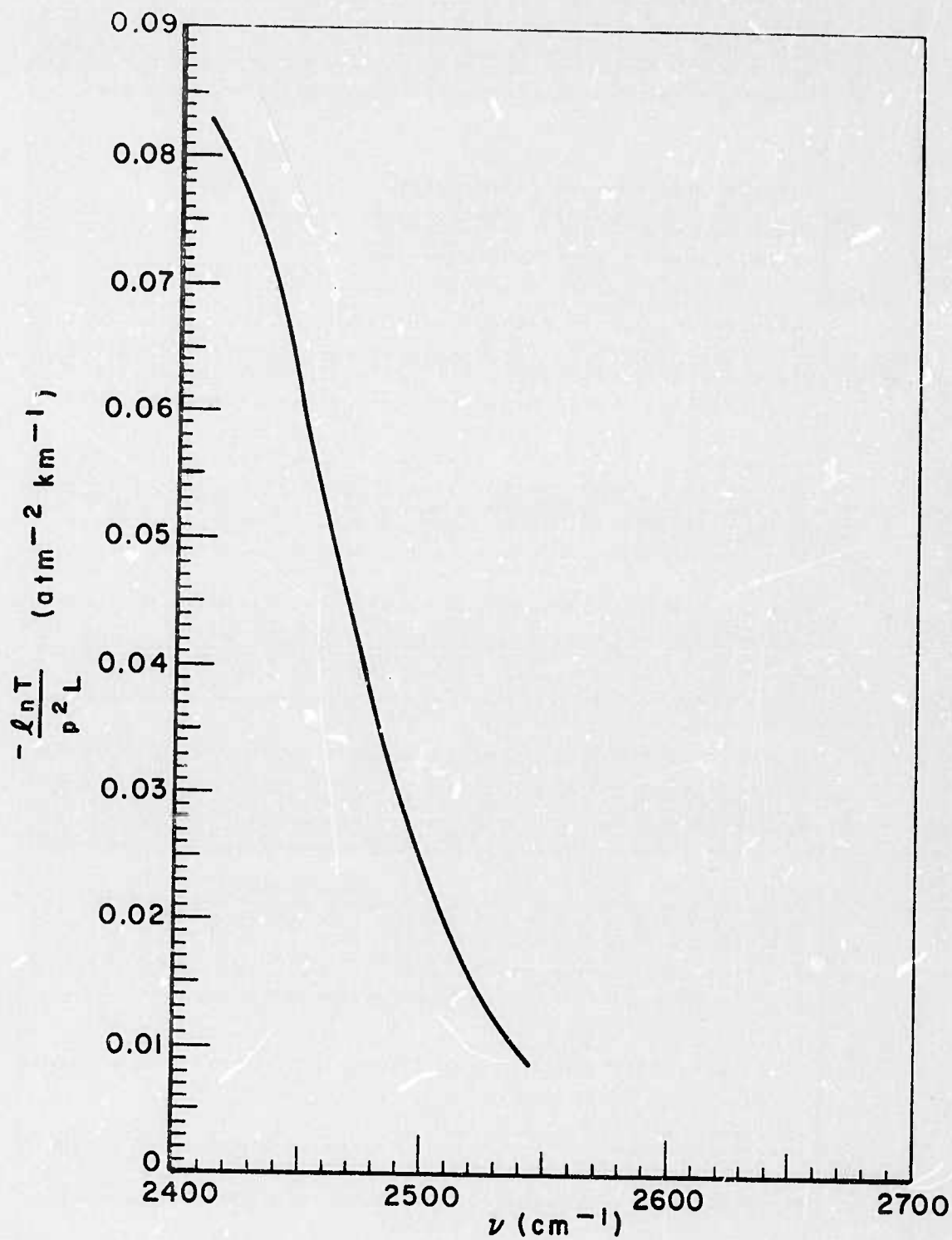


Fig. ii. Nitrogen absorption from Fig. 4 of  
AFCRL 73-0096,  $T = 296^\circ \text{K}$ .



TABLE III  
Mid-Latitude Summer Sea Level Absorption Coefficients  
Calculated from AFCRL Absorption Line-Data

Line	Iden	S*	N <sub>2</sub> O	CH <sub>4</sub>	CO <sub>2</sub>	H <sub>2</sub> O	H <sub>2</sub> O Cont	N <sub>2</sub>	Total
2445.41	3-2,12	c	2.519E-3	4.268E-9	1.042E-2	3.095E-5	2.85E-2	6.6E-2	1.075E-1
2471.29	3-2,11	c	4.087E-3	7.683E-8	3.713E-5	4.997E-3	2.52E-2	4.6E-2	8.032E-2
2496.77	3-2,10	c	8.055E-4	1.109E-5	5.381E-8	6.540E-4	2.27E-2	2.5E-2	4.917E-2
2500.48	2-1,13	b	7.635E-3	2.881E-6	2.735E-8	1.267E-4	2.22E-2	2.5E-2	5.496E-2
2521.81	3-2,9	c	4.511E-4	2.748E-6	2.094E-7	2.321E-4	2.05E-2	1.5E-2	3.619E-2
2527.42	2-1,12	b	8.387E-4	1.841E-5	1.814E-7	2.539E-4	2.00E-2	1.4E-2	3.511E-2
2546.42	3-2,8	c	1.399E-2	1.833E-3	1.196E-7	1.347E-3	1.86E-2	8.0E-3	4.377E-2
2553.97	2-1,11	b	9.655E-3	7.757E-5	1.036E-7	5.113E-4	1.82E-2	7.1E-3	3.554E-2
2570.51	3-2,7	a	3.367E-2	3.174E-5	7.826E-8	4.783E-3	1.75E-2	5.0E-3	6.098E-2
2580.10	2-1,10	b	4.458E-2	2.618E-6	6.763E-8	2.684E-3	1.70E-2	3.6E-3	6.787E-2
2583.47	1-0,13	b	2.517E-2	5.008E-6	6.441E-8	3.580E-3	1.69E-2	3.45E-3	4.91E-2
2594.25	3-2,6	c	1.954E-3	1.612E-5	5.553E-8	6.666E-3	1.68E-2	2.6E-3	2.804E-2
2605.80	2-1,9	b	5.362E-4	2.046E-4	4.792E-8	1.937E-2	1.68E-2	2.3E-3	3.921E-2
2611.14	1-0,12	b	9.147E-5	3.795E-6	4.492E-8	8.245E-3	1.70E-2	2.1E-3	2.744E-2
2617.44	3-2,5	c	1.170E-5	7.513E-5	4.174E-8	2.872E-3	1.72E-2	2.0E-3	2.216E-2
2631.06	2-1,8	b	1.229E-7	7.884E-4	3.591E-8	1.476E-2	1.78E-2	1.9E-3	3.525E-2
2638.39	1-0,11	b	1.271E-8	5.999E-4	3.327E-8	2.472E-1	1.82E-2	1.6E-3	2.676E-1
2655.85	2-1,7	b	1.103E-11	6.015E-4	2.805E-8	7.905E-2	1.93E-2		9.895E-2
2665.22	1-0,10	b	1.418E-11	1.975E-3	2.573E-8	1.512E-2	2.00E-2		3.709E-2
2680.17	2-1,6	b	2.291E-11	3.103E-4	2.260E-8	3.689E-2	2.12E-2		5.84E-2
2691.61	1-0,9	b	3.647E-11	3.223E-3	2.057E-8	5.509E-2	2.20E-2		8.03E-2
2703.99	2-1,5	b	7.099E-11	2.073E-6	1.867E-8	5.454E-3	2.30E-2		2.846E-2
2717.54	1-0,8	b	2.441E-9	2.335E-6	1.688E-8	8.986E-2	2.41E-2		1.14E-1
2727.30	2-1,4	b	2.679E-8	1.475E-4	1.574E-8	4.248E-2	2.51E-2		6.773E-2
2743.00	1-0,7	b	4.321E-6	2.850E-4	1.414E-8	3.300E-2	2.69E-2		6.019E-2
2750.09	2-1,3	b	4.062E-5	8.969E-4	1.350E-8	1.255E-2	2.75E-2		4.099E-2
2767.97	1-0,6	b	1.029E-4	4.949E-3	1.206E-8	5.130E-2	3.08E-2		8.715E-2
2792.43	1-0,5	b	8.076E-4	6.103E-4	1.044E-8	3.732E-2	3.50E-2		7.374E-2
2816.38	1-0,4	b	1.158E-3	2.859E-3	9.144E-9	6.043E-2	4.00E-2		1.044E-1
2839.78	1-0,3	b	4.945E-7	7.241E-4	8.100E-9	5.749E-2	4.50E-2		1.032E-1

\*Source of laser line data

a - Mills (OSU)

b - calculated from molecular constants (P.K.L. Yin, OSU Physics Dept.)

c - Deutsch (7)

There is also a remarkable uniformity in the calculated coefficients for 29 of the 30 laser lines, the exception being the 1-0<sub>11</sub> line at 2638.39 cm<sup>-1</sup>. The laser lines miss all of the regions of intense absorption. This fortunate situation will also be clear from an examination of the plots to be given in a later section.

Table IV shows the output spectrum of a 200 watt DF laser which

TABLE IV  
Distribution of Power for TRW 200 Watt DF Laser  
Including Mid-Latitude Summer Absorption  
Coefficient from Table III

Line	Iden	Percent	Coefficient
2496.77	3-2,10	.8	
2521.81	3-2,9	3.6	
2546.42	3-2,8	2.6	
2570.51	3-2,7	12.8	.061
2580.10	2-1,10	2.6	
2594.25	3-2,6	4.3	
2605.80	2-1,9	5.6	
2617.44	3-2,5	.8	
2631.06	2-1,8	12.3	.0353
2655.85	2-1,7	11.3	.099
2680.17	2-1,6	12.8	.0584
2691.61	1-0,9	.5	
2703.99	2-1,5	1.0	
2717.54	1-0,8	4.0	
2743.00	1-0,7	4.1	
2767.97	1-0,6	6.1	
2792.43	1-0,5	4.1	
		100.0	

was constructed at TRW, Inc. Fifty percent of the total power is obtained on four lines: 3-2<sub>7</sub> and 2-1<sub>6</sub>, 2-1<sub>7</sub>, and 2-1<sub>8</sub>. For the 3-2<sub>7</sub> line 84 percent of the absorption is caused by N<sub>2</sub>O and N<sub>2</sub> with N<sub>2</sub>O being the most important. For the above 2-1 lines from 86 to 99% of the absorption is due to water vapor.

Table V shows the spectrum of the TRW propagation test laser and the predicted absorption coefficients from Table III.

TABLE V  
DF Laser Calculated Absorption Coefficients for Mid-Latitude  
Summer Sea Level Model with Normalized Relative  
Intensities of DF Lines in TRW Propagation  
Test Laser (3 cm Active Length).

Iden	Freq ( $\text{cm}^{-1}$ )	Normalized Relative Intensity	Absorption Coefficient ( $\text{km}^{-1}$ )
4-3,7		.08	
3-2,10	2496.77	.045	.0492
4-3,6		.163	
3-2,9	2521.81	.102	.0362
4-3,5		.08	
3-2,8	2546.42	.364	.0438
3-2,7	2570.51	.489	.061
2-1,10	2580.10	.07	.0679
3-2,6	2594.25	.688	.028
2-1,9	2605.80	.244	.0392
3-2,5	2617.44	.432	.022
2-1,8	2631.06	.648	.0353
2-1,7	2655.85	.693	.099
2-1,6	2680.17	1.00	.058
1-0,9	2691.61	.248	.080
2-1,5	2703.99	.307	.0285
1-0,8	2717.54	.494	.114
1-0,7	2743.00	.670	.0602
1-0,6	2767.97	.642	.087
1-0,5	2792.43	.21	.0737

#### IV. PLOTS

In order to provide additional insight into the molecular absorption problem, plots of  $\text{N}_2\text{O}$ ,  $\text{CH}_4$ , and water vapor absorption were also prepared.

The water vapor plots do not include the water continuum of Fig. i. The water plots are for 15 torr  $\text{H}_2\text{O}$  at  $294^\circ\text{K}$ , i.e., a relative humidity of 80 percent, a total pressure of 760 torr and a path length of 10 km. The laser wavelengths of Table III are clearly marked.

In all 54 plots were made. Figures 1-18 are the CH<sub>4</sub> plots. The path length was one km in all cases. The CH<sub>4</sub> pressure was varied from 0.1 to 30.0 torr to produce an onscale plot. Note from Table I that these partial pressures are all much greater than the  $1.3 \times 10^{-3}$  torr assumed in the sea level model atmosphere. The plots are mostly useful in examining the nature of the spectrum in the vicinity of the DF laser wavelengths in order to estimate which absorption coefficients from Table III may be in error due to incorrect data on either the absorption line or laser line positions. For example, see the 3-2 P(8) line, Fig. 3; 2-1 P(9), Fig. 5; 2-1 P(7), Fig. 8; 2-1 P(3), Fig. 14; etc. It is interesting also to examine the plots for the four high power laser lines given in Table IV.

Figures 19-35 give the plots for N<sub>2</sub>O. Again the path length was one km and the partial pressure was from .002-30 torr as compared to the sea level model which contains  $2.3 \times 10^{-4}$  torr N<sub>2</sub>O.

Figures 36-54 give the water vapor plots. In this case the path length was increased to 10 km and the partial pressure was maintained at 15 torr.

Experiments are being undertaken at Ohio State University where DF laser sources are being used together with a one km multitraversal absorption cell or an acoustic spectrophone in order to obtain direct information as to the accuracy of the predictions which have been given in this report.

## V. COMPARISON TO AFCRL CALCULATIONS

We have attempted to compare our results with those reported earlier by McClatchey[2]. First, the calculations presumably use the same input line-data, namely the AFCRL GOAT tape[1]. Nevertheless differences in the results were noted which presumably must be due to differences in some of the other variables. There are some differences in approach where one cannot say that one is correct and the other not. Also we have not had a copy of Dr. McClatchey's computer program so that we are not entirely sure that the information given below is correct. Nevertheless from a study of some of the AFCRL reports[1,2] we have concluded that for the measurements reported in AFCRL-72-0312 the following data was used:

BOUND = 20 cm<sup>-1</sup>  
BX as in Table II  
CX = 0.5 all gases  
Mid-Latitude Summer Model as in Table I  
Lorentz line shape  
B = 1.0 all gases.

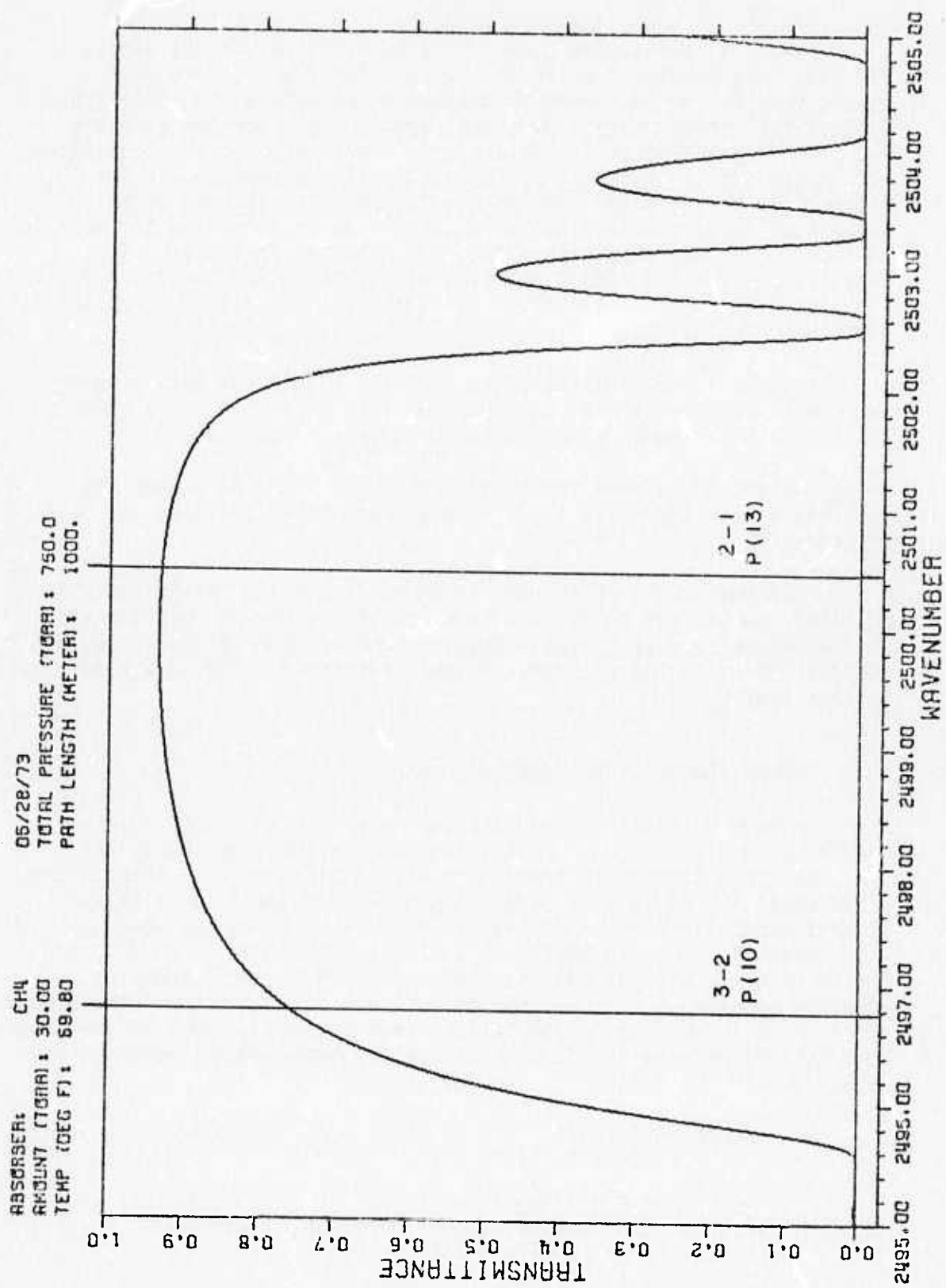


Fig. 1



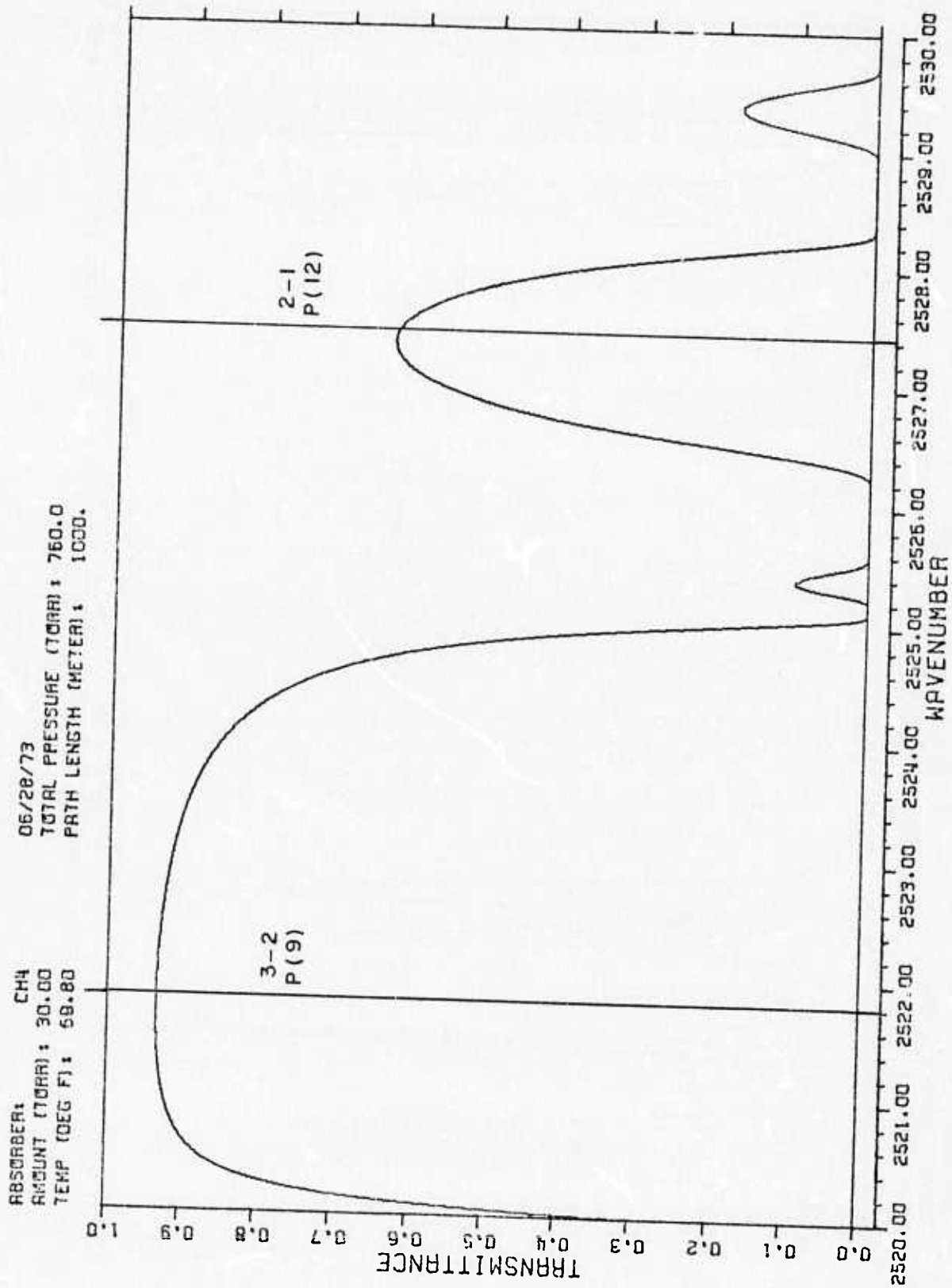


Fig. 2



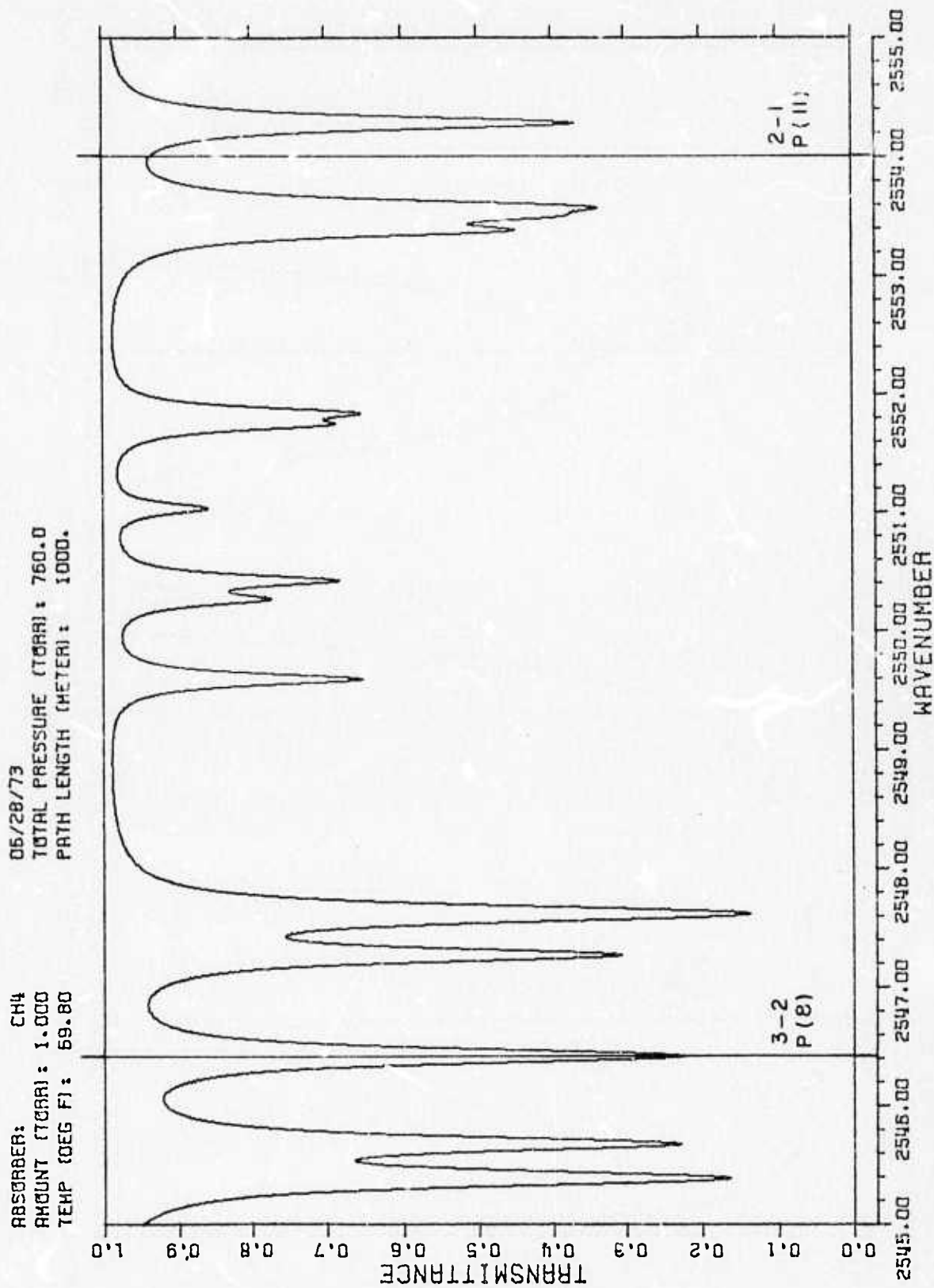


Fig. 3

ABSORBER: CH<sub>4</sub>  
AMOUNT (TORR): 10.00  
TEMP (DEG F): 69.60

06/28/73  
TOTAL PRESSURE (TORR): 760.0  
PATH LENGTH (METER): 1000.

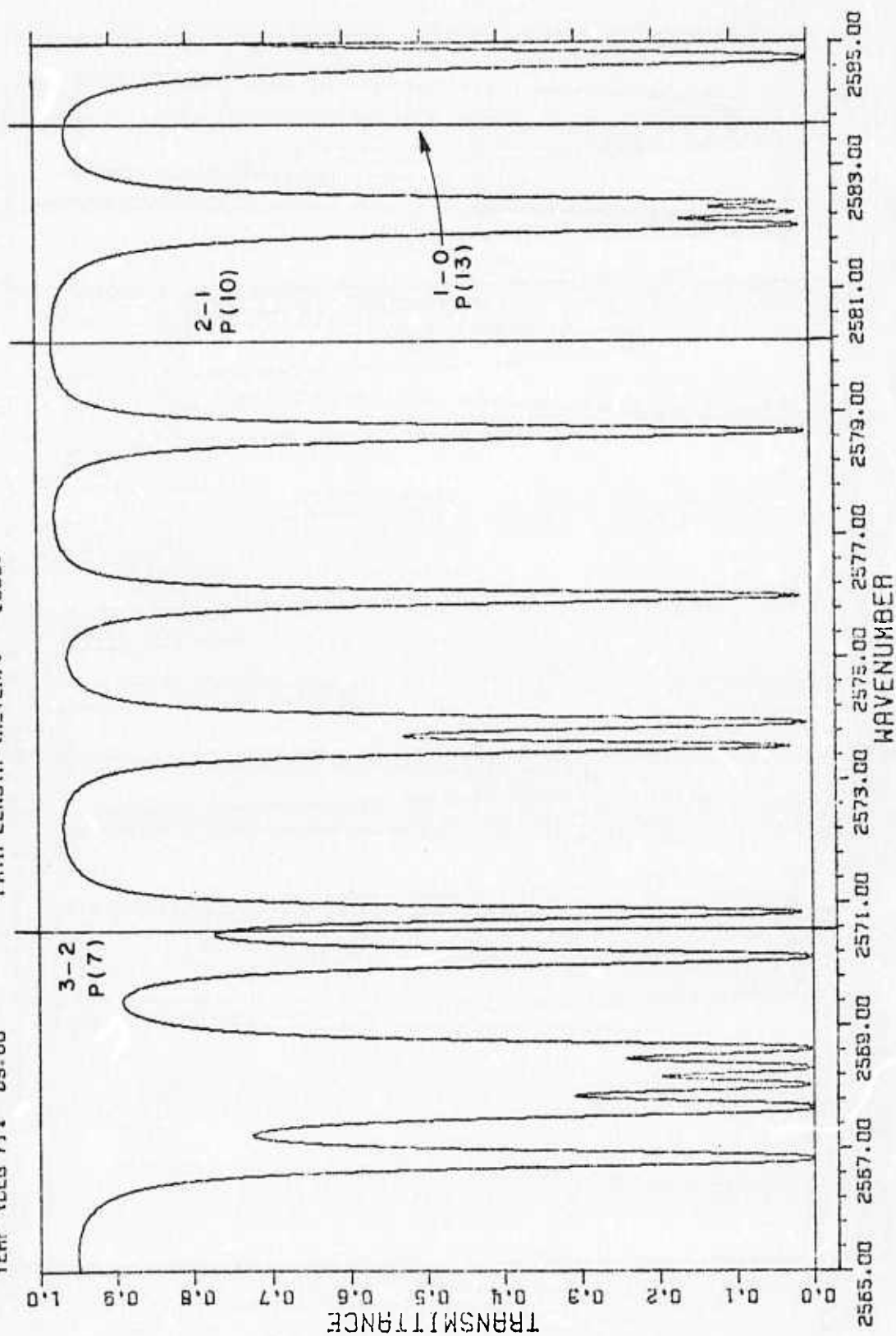


Fig. 4

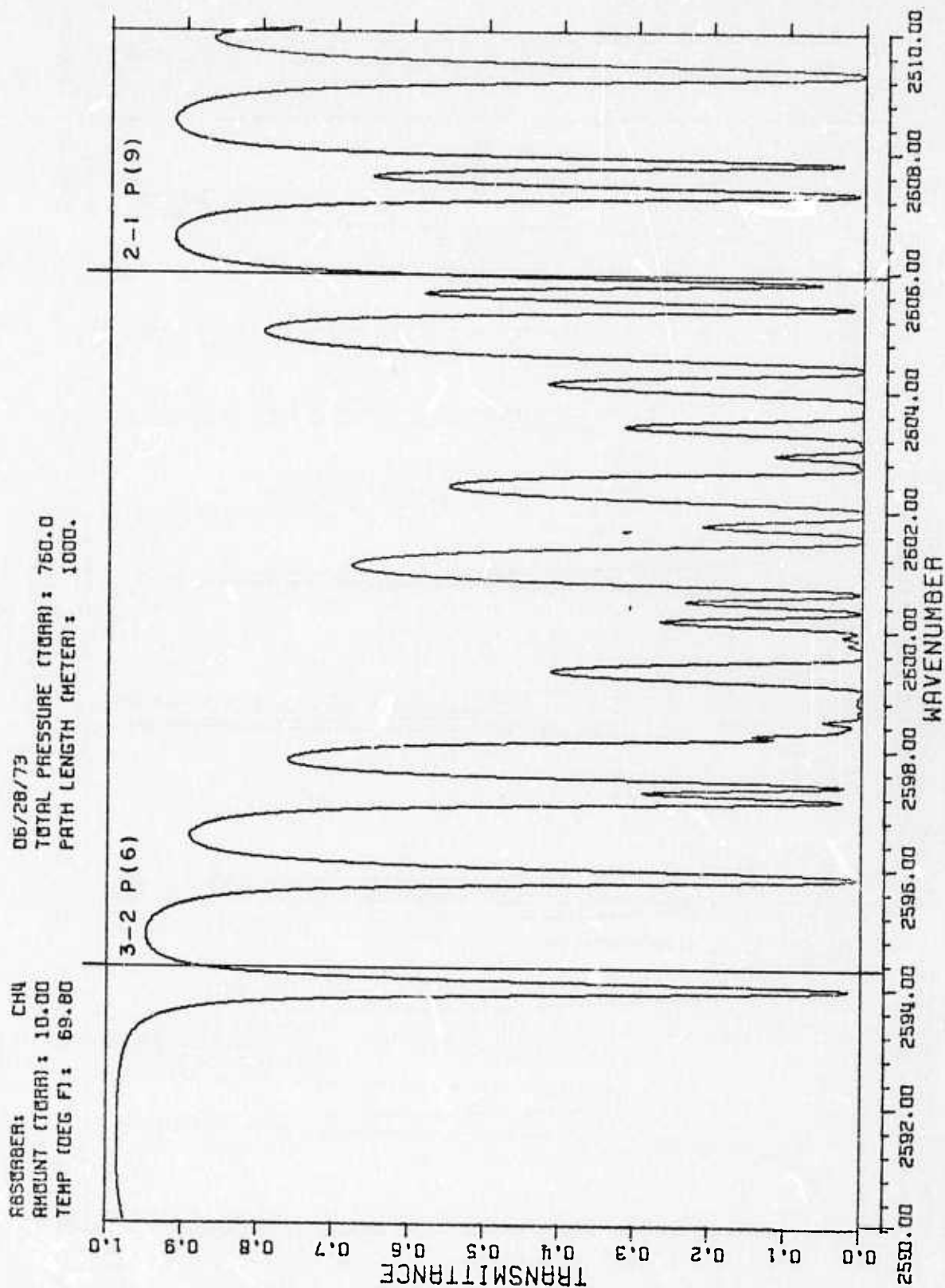


Fig. 5

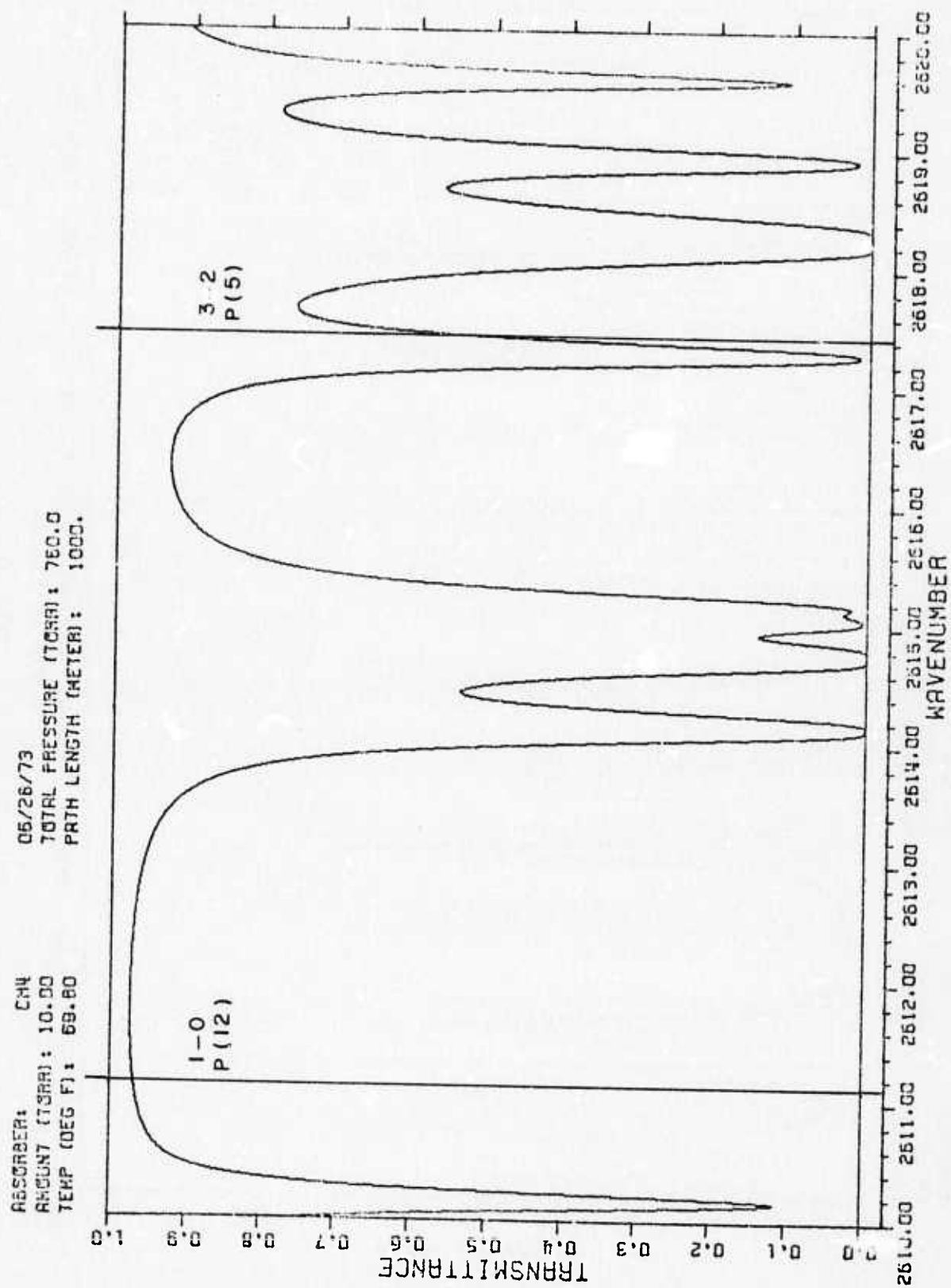


Fig. 6

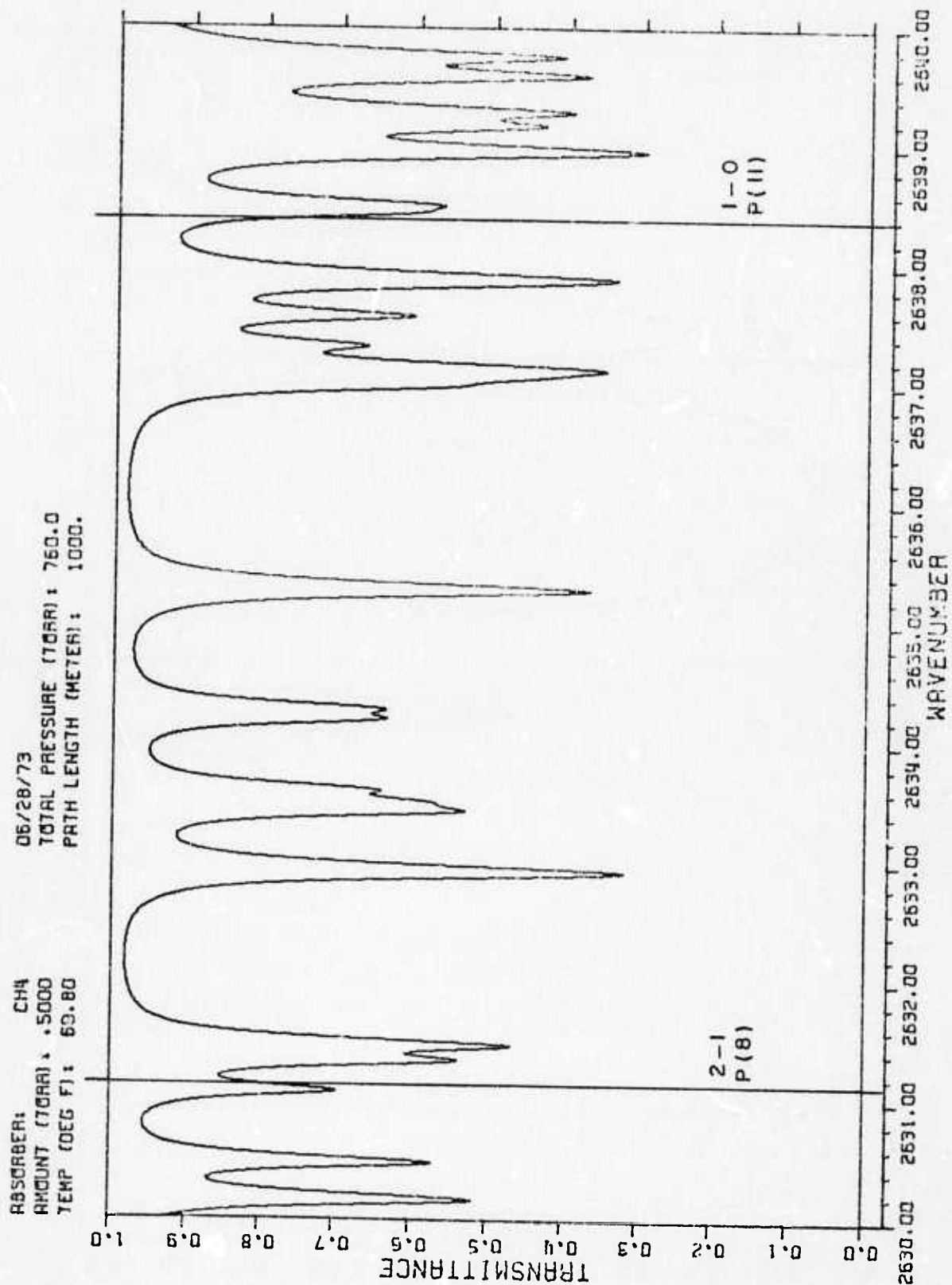


Fig. 7

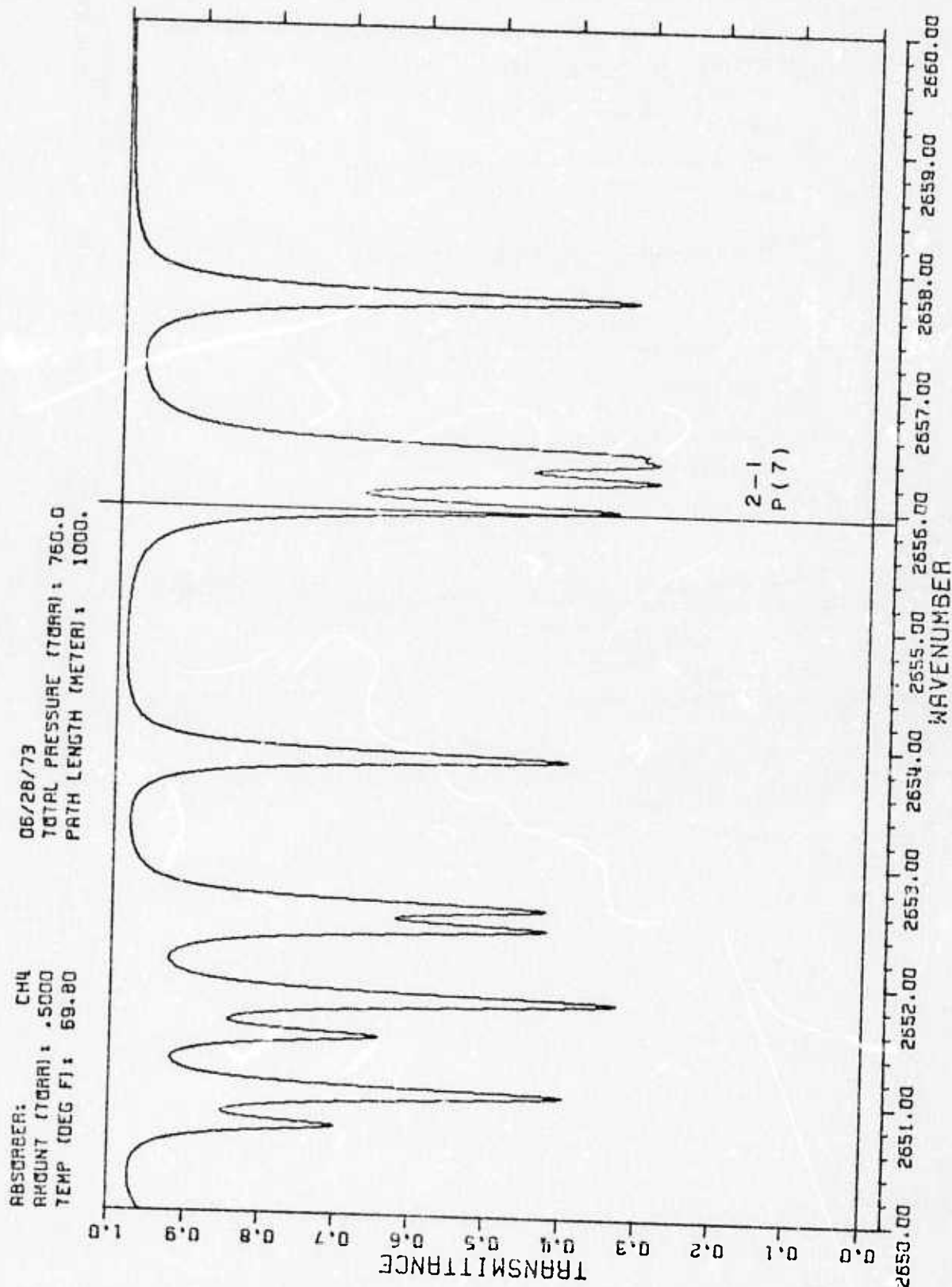


Fig. 8



06/28/73  
TOTAL PRESSURE (TORR): 760.0  
PATH LENGTH (METER): 1000.

ABSORBER: CH4  
AMOUNT (TORR): .5000  
TEMP (DEG F): 69.80

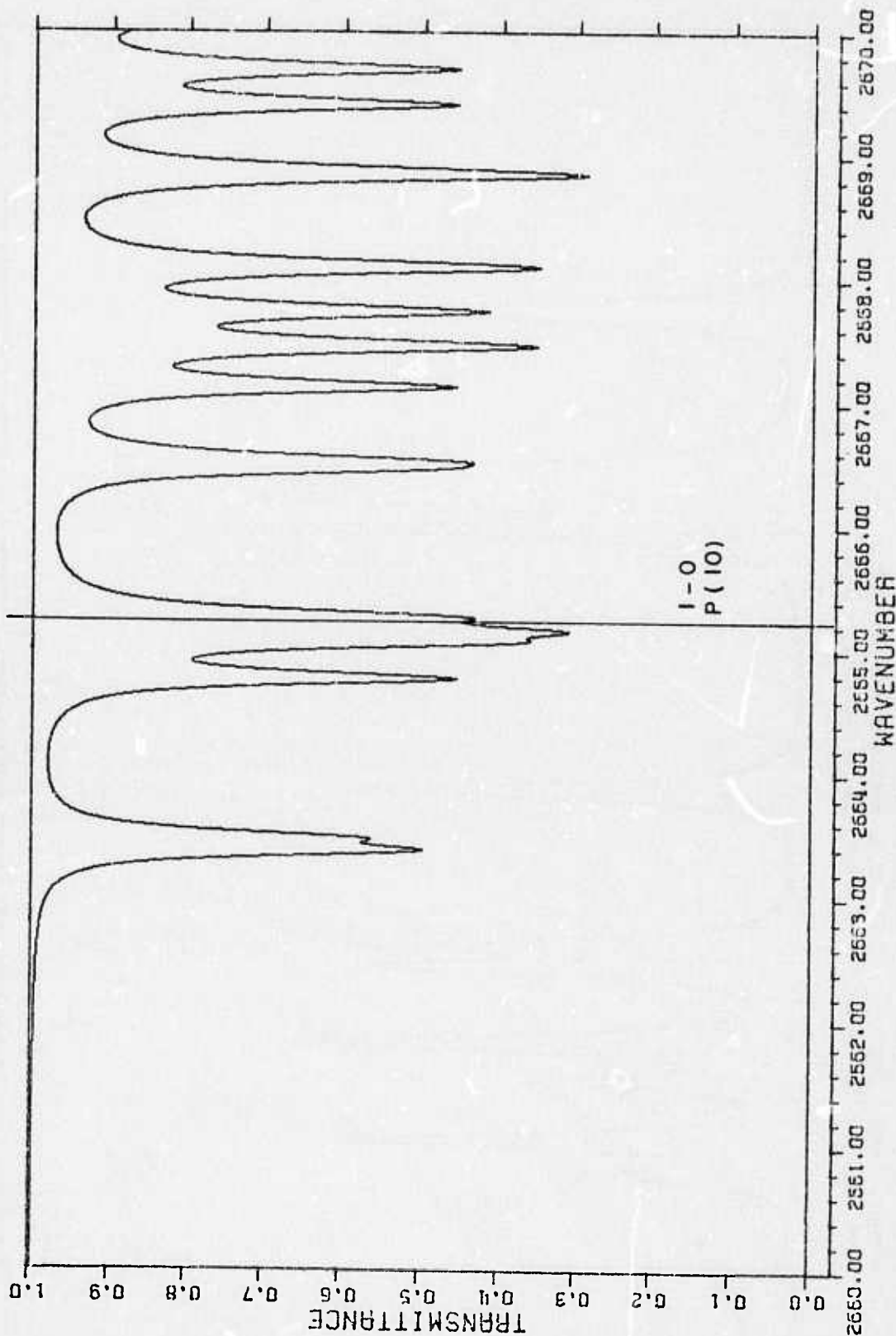


Fig. 9

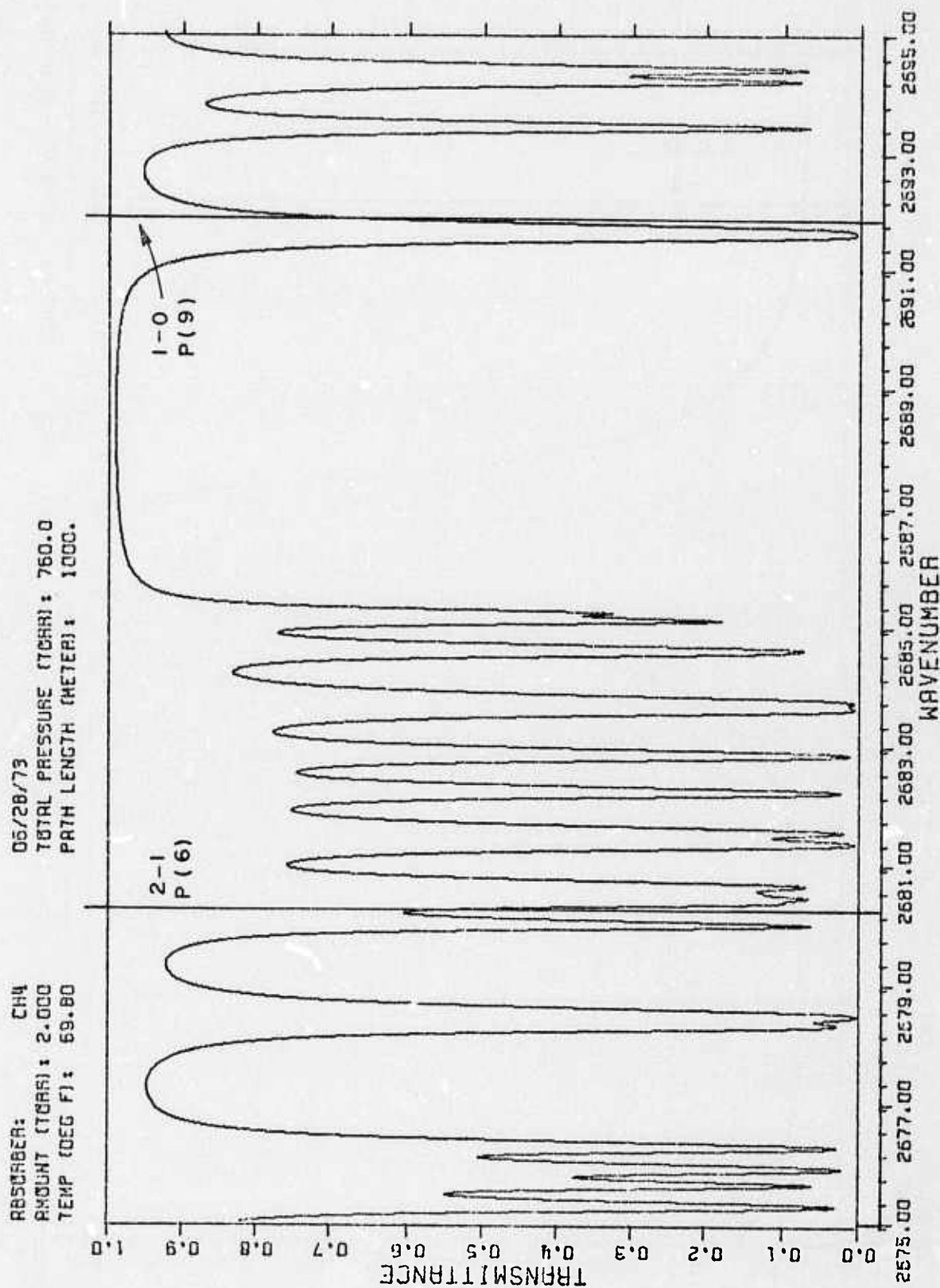


Fig. 10

ABSORBER: CH<sub>4</sub>  
AMOUNT (TORR): 30.00  
TEMP (DEG F): 69.80

06/28/73  
TOTAL PRESSURE (TORR): 760.0  
PATH LENGTH (METER): 1000.

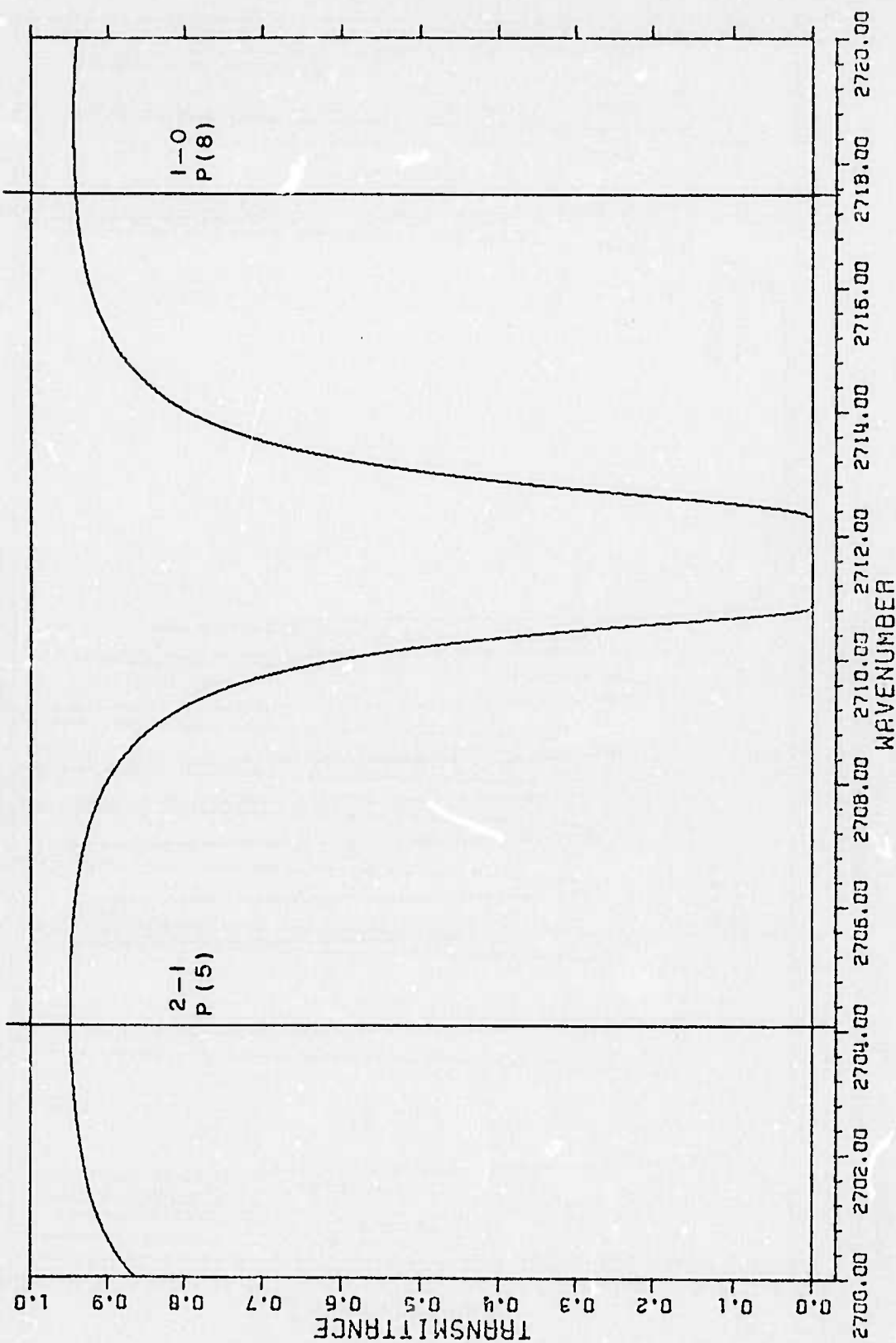


Fig. 1

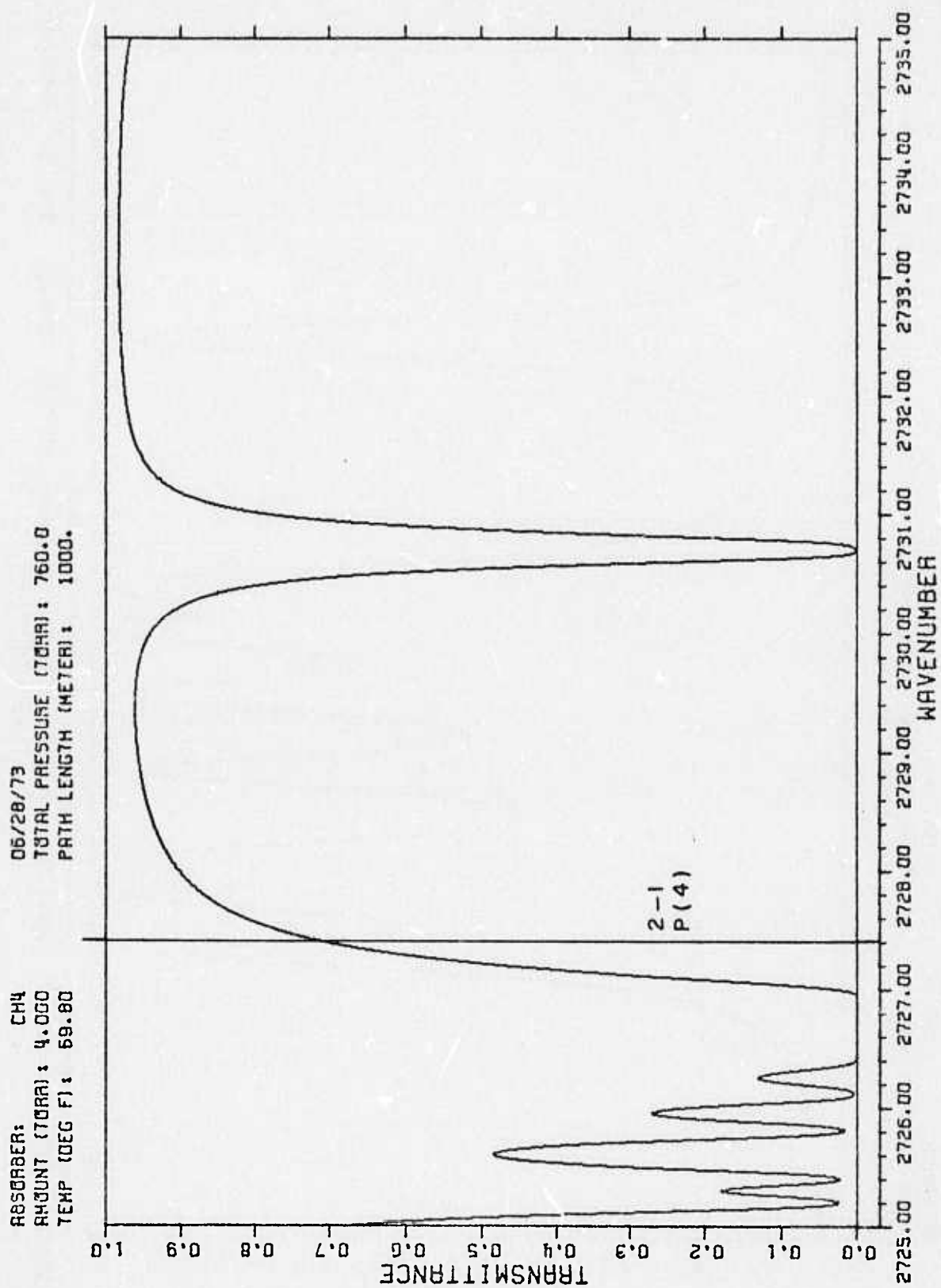


Fig. 12

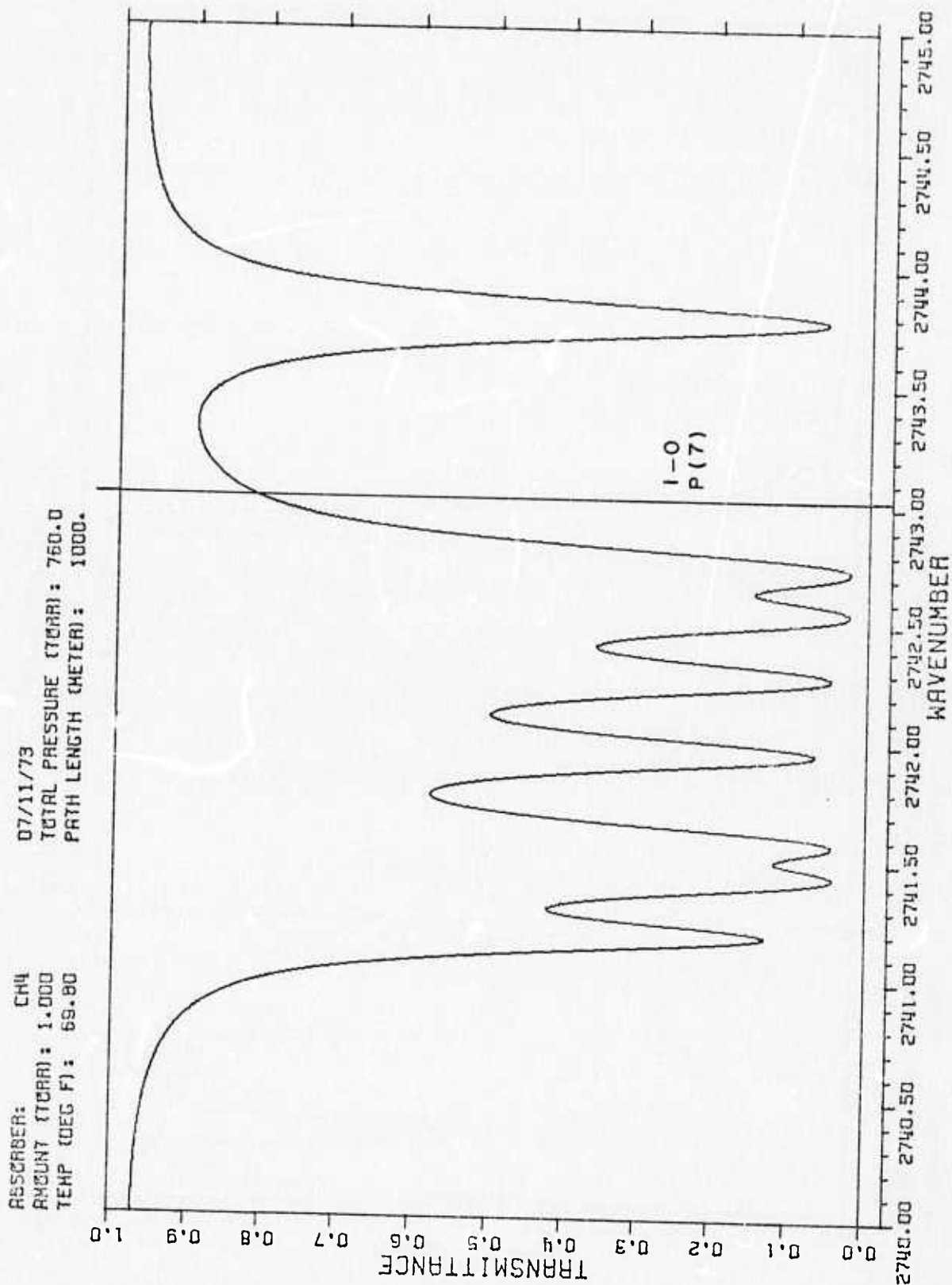


Fig. 13

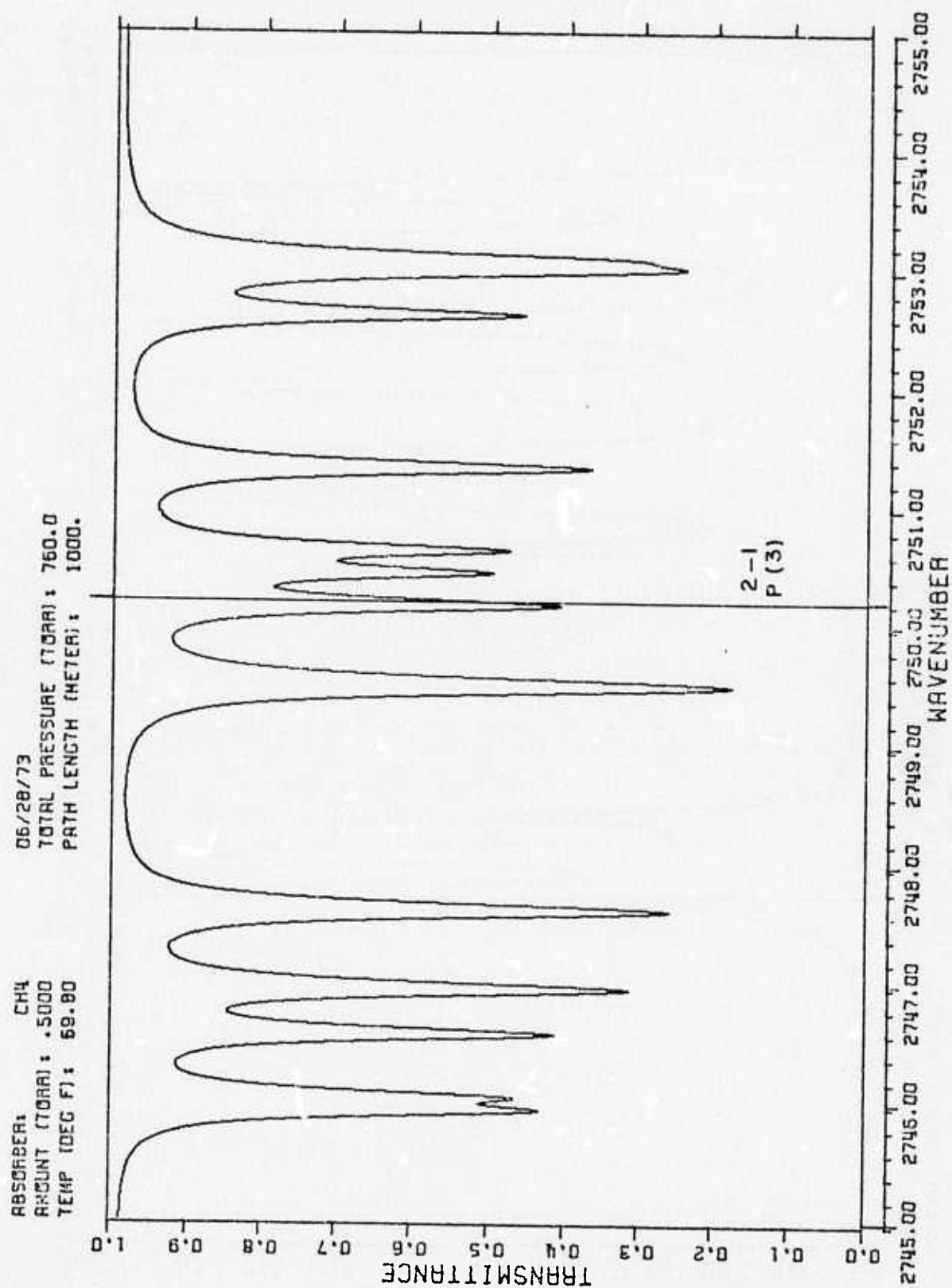


Fig. 14



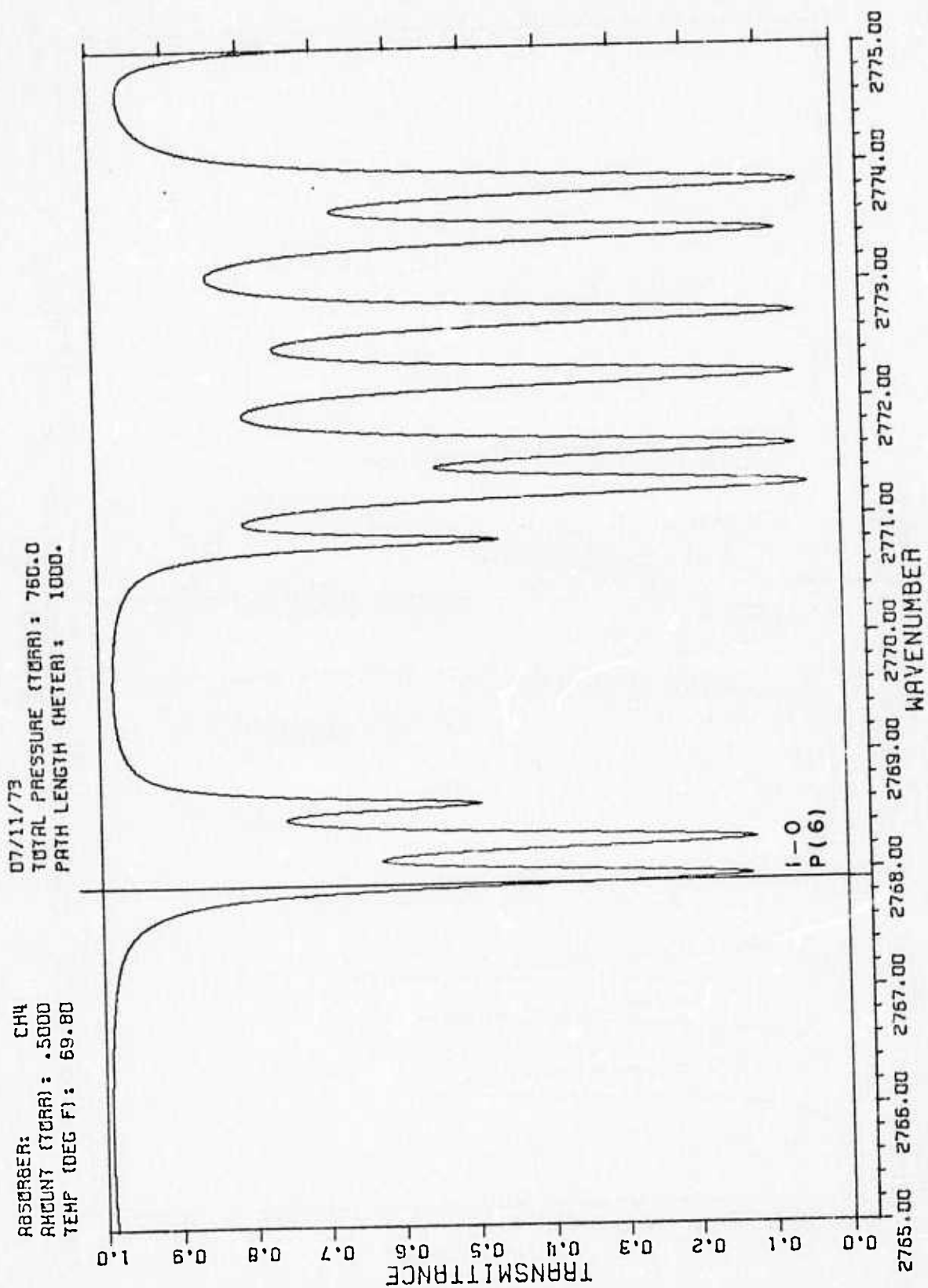


Fig. 15

ABSORBER: CH4  
AMOUNT (TORR): 1.000  
TEMP (DEG F): 69.80

07/13/73  
TOTAL PRESSURE (TORR): 760.0  
PATH LENGTH (METER): 1000.

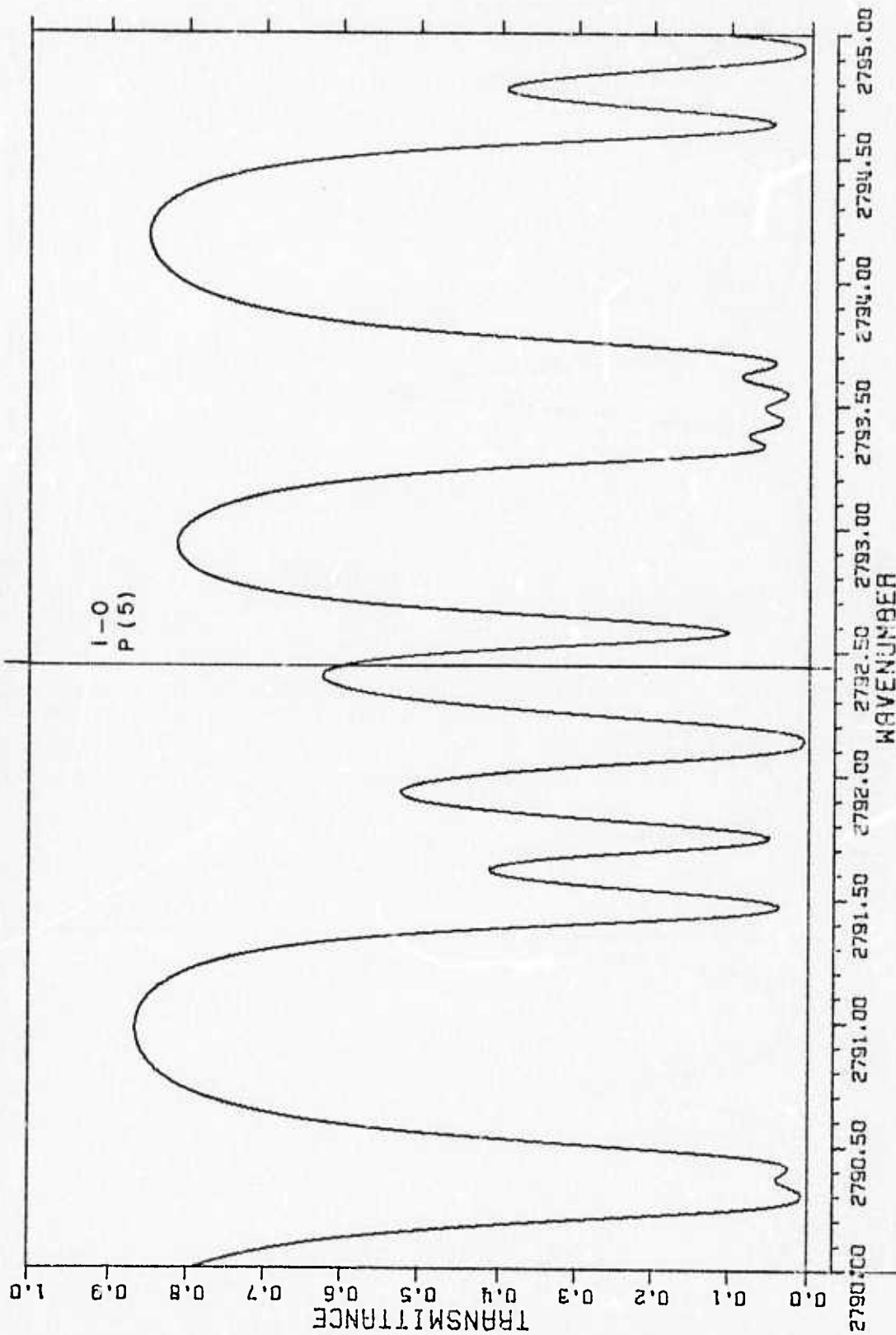


Fig. 16

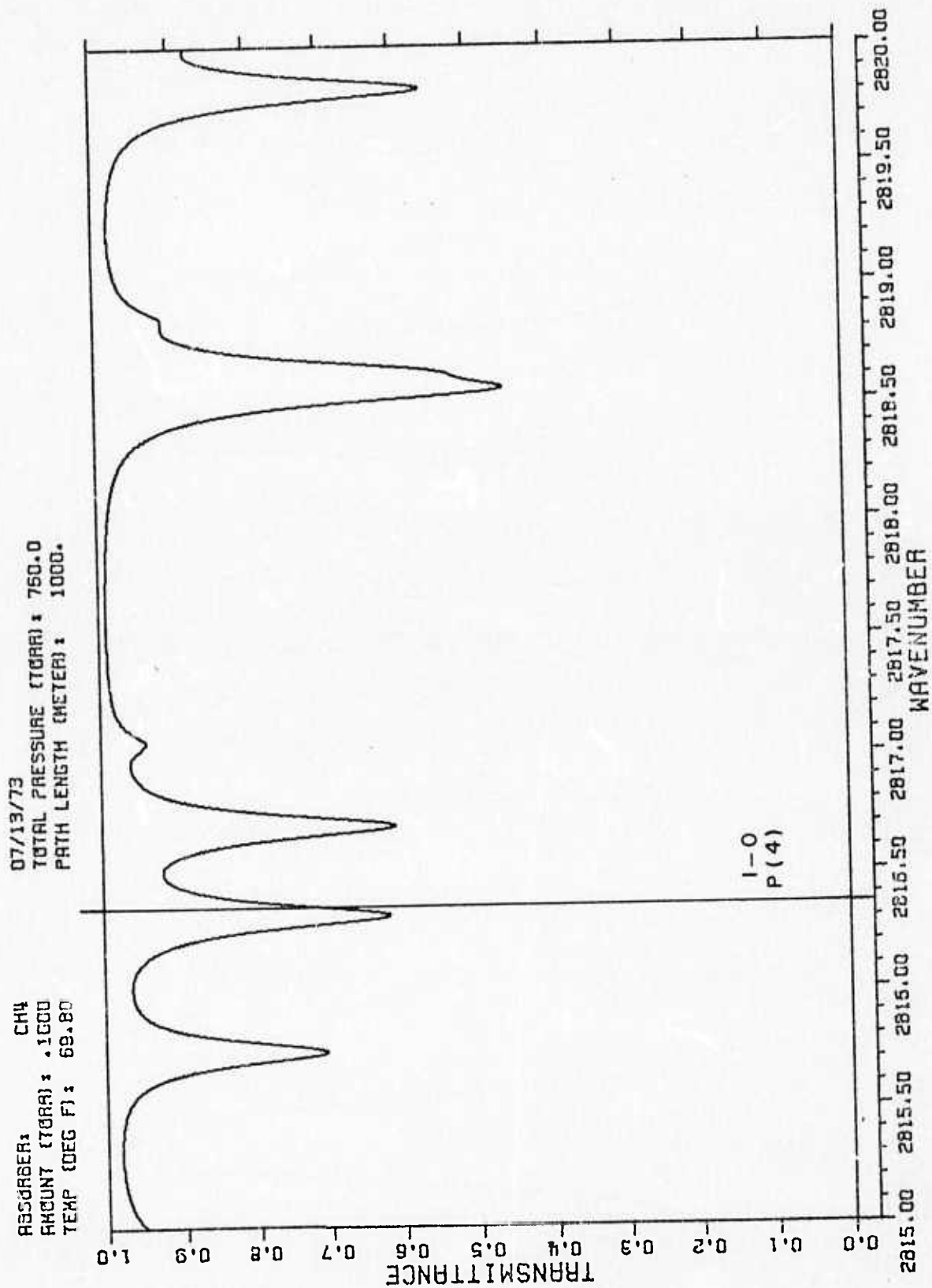


Fig. 17

RECORDER: CH4  
PUNCT (TORR): 1.000  
TEMP (DEG F): 69.80

07/13/73  
TOTAL PRESSURE (TORR): 760.0  
PATH LENGTH (METER): 1000.

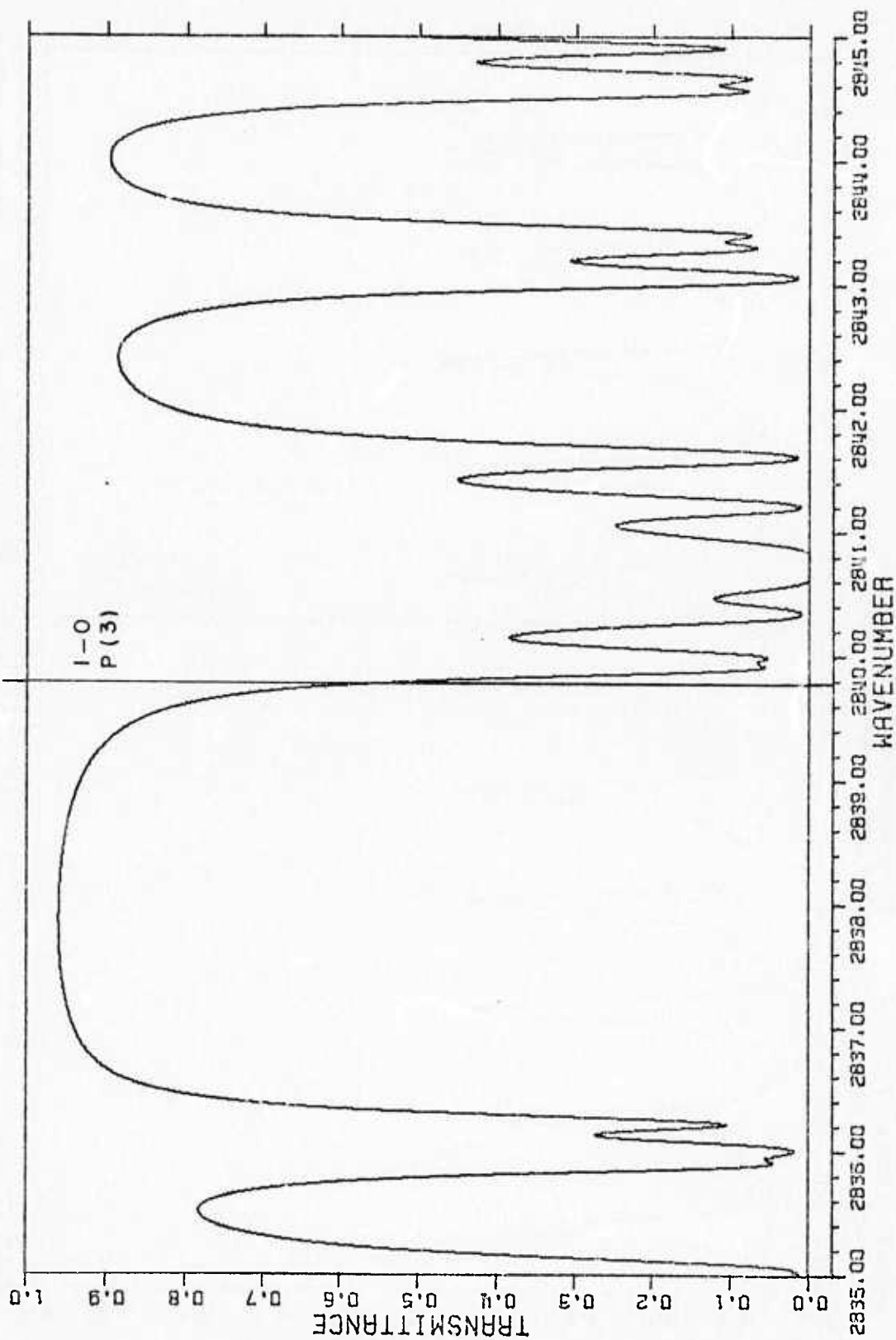


Fig. 18

ABSORBER: N2O  
AMOUNT (TORR): .0100  
TEMP (DEG F): 69.80

06/28/73  
TOTAL PRESSURE (TORR): 750.0  
PATH LENGTH (METER): 1000.

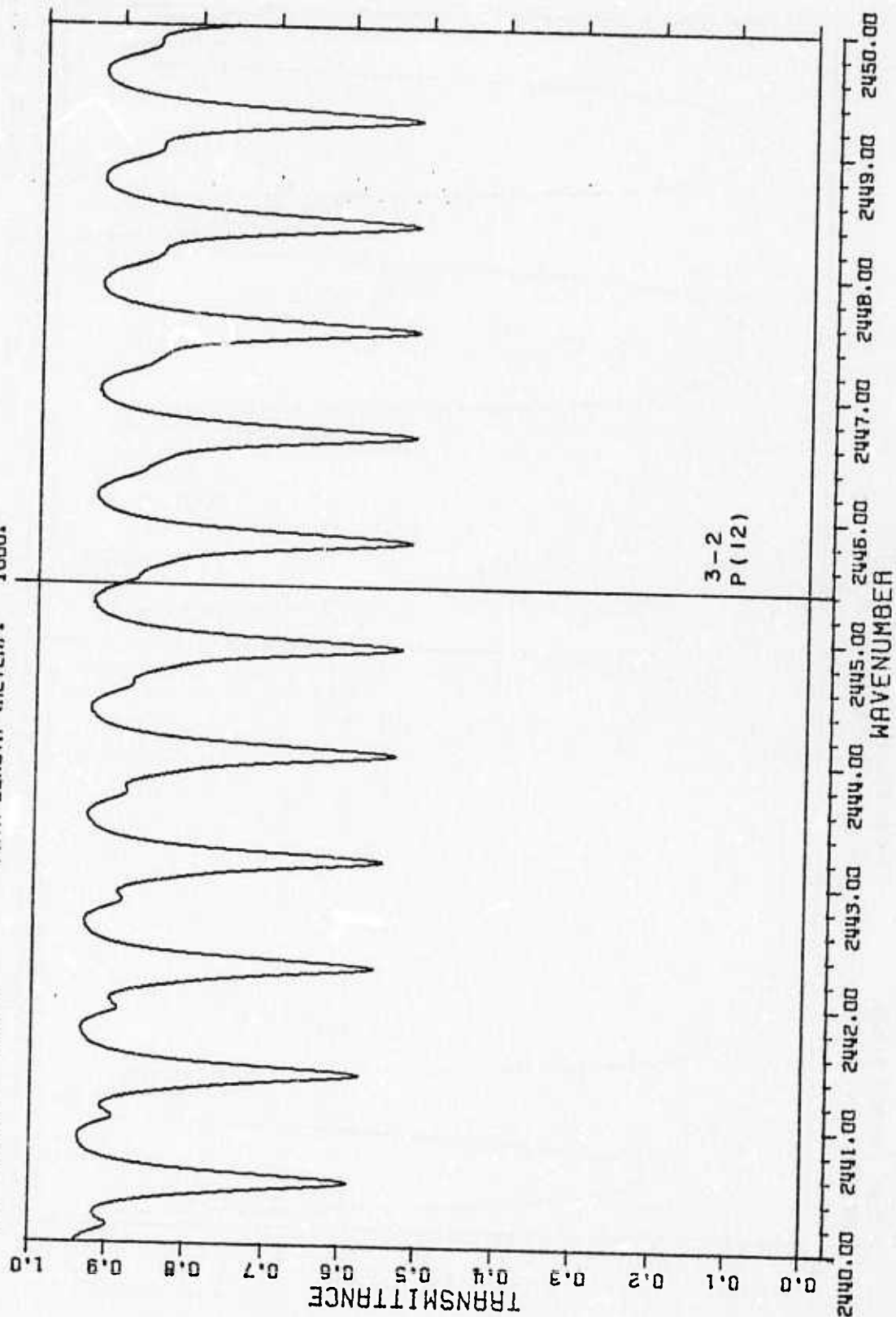


Fig. 19

ABSORBER: N2O  
AMOUNT (TORR): .0100  
TEMP (DEG F): 69.60

06/28/73  
TOTAL PRESSURE (TORR): 760.0  
PATH LENGTH (METER): 1000.

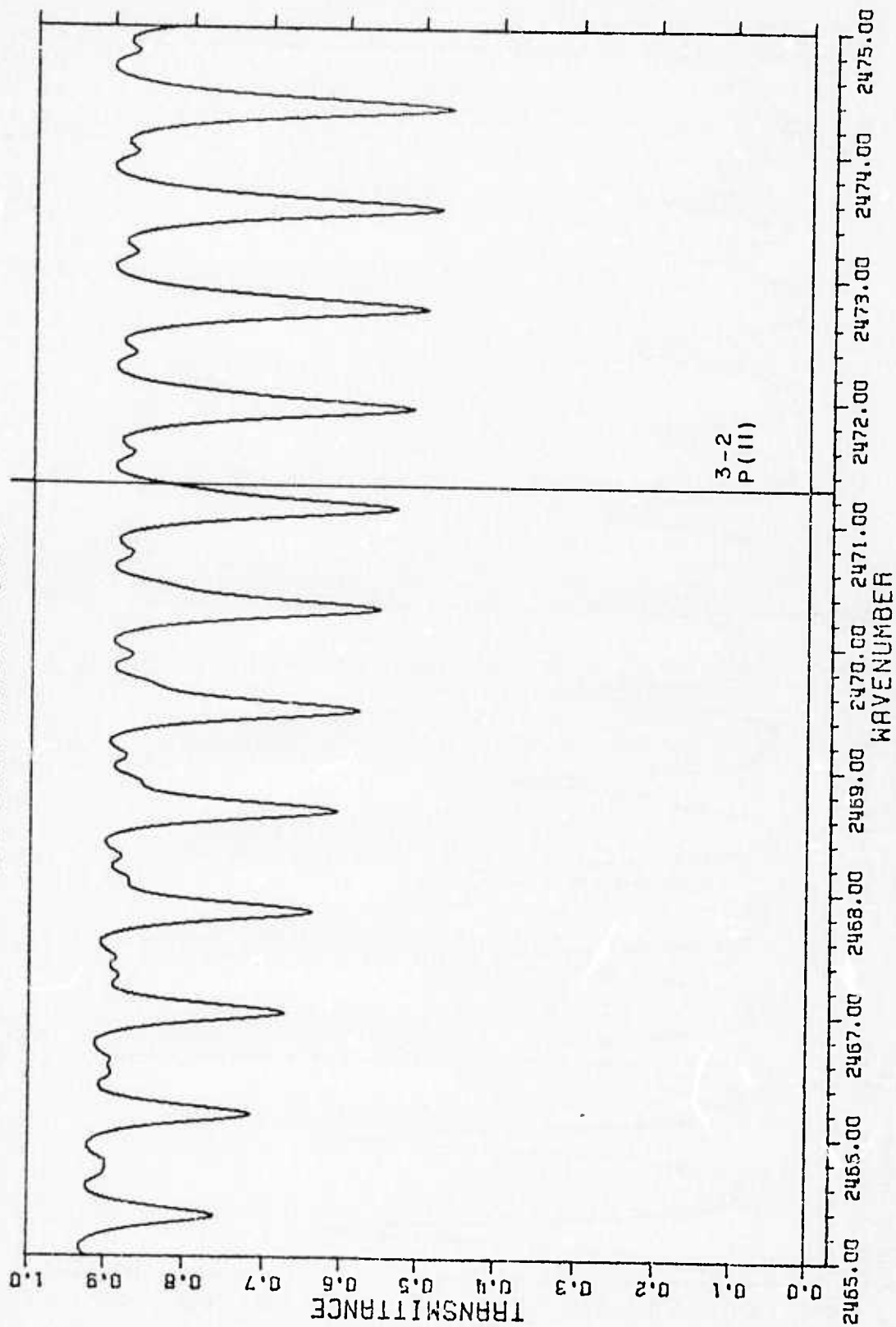


Fig. 20



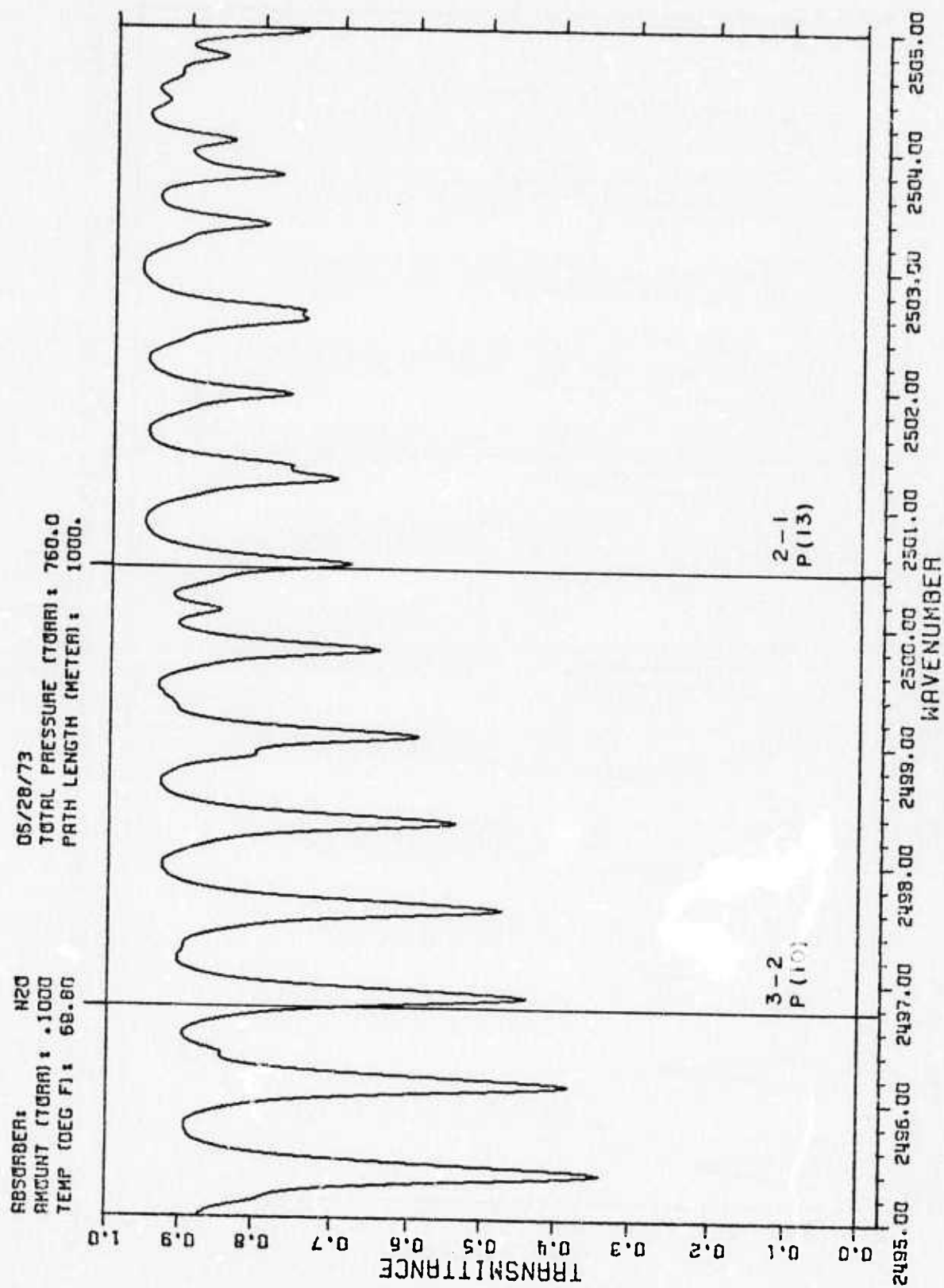


Fig. 21

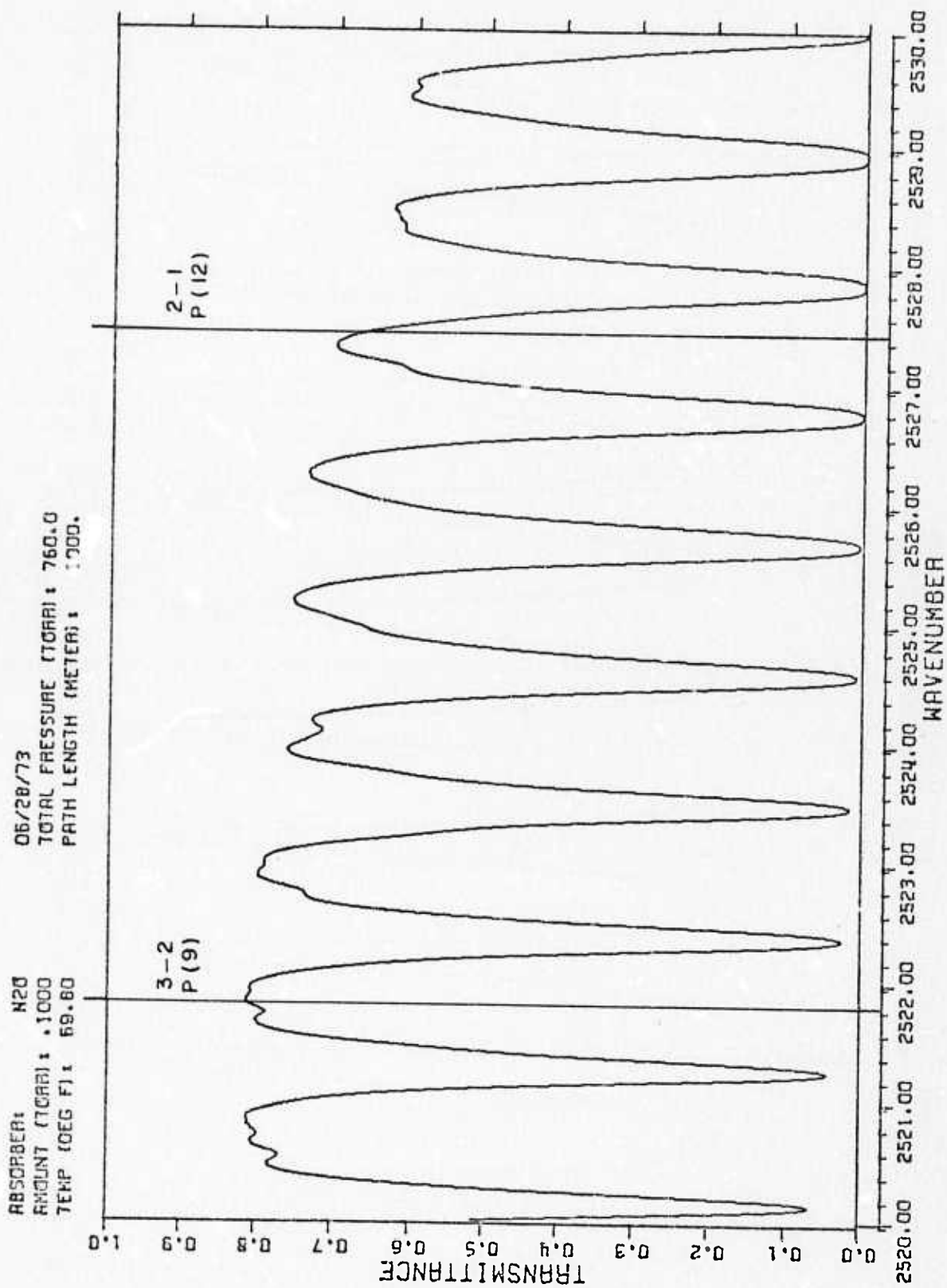


Fig. 22

ABSORBER: N<sub>2</sub>O  
AMOUNT (TORR): .0100  
TEMP (DEG F): 59.80

06/28/73  
TOTAL PRESSURE (TORR): 760.0  
PATH LENGTH (METER): 1000.

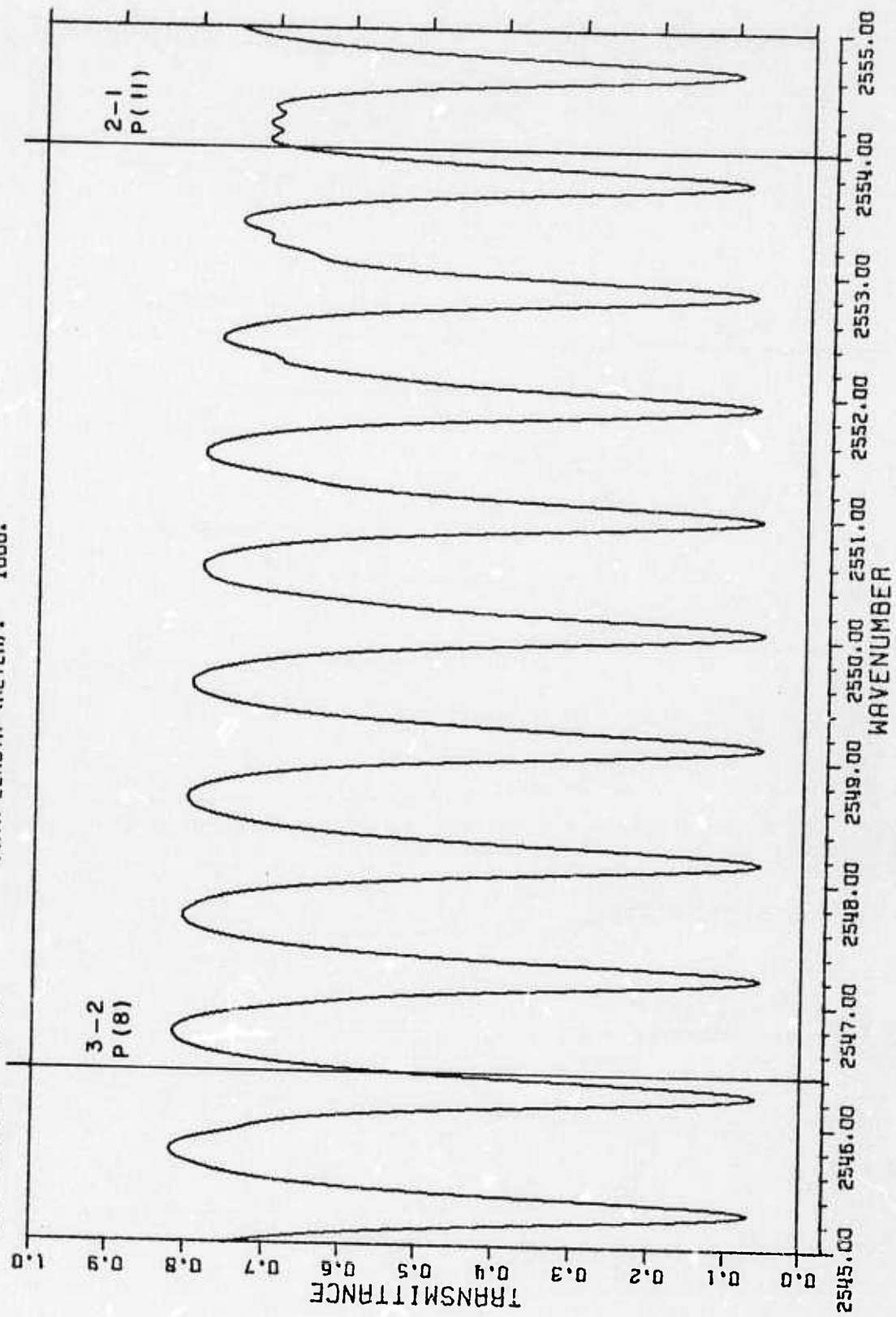


Fig. 23

ABSORBER: N2O  
AMOUNT (TORR): .0020  
TEMP (DEG F): 69.00

06/28/73  
TOTAL PRESSURE (TORR): 760.0  
PATH LENGTH (METER): 1000.

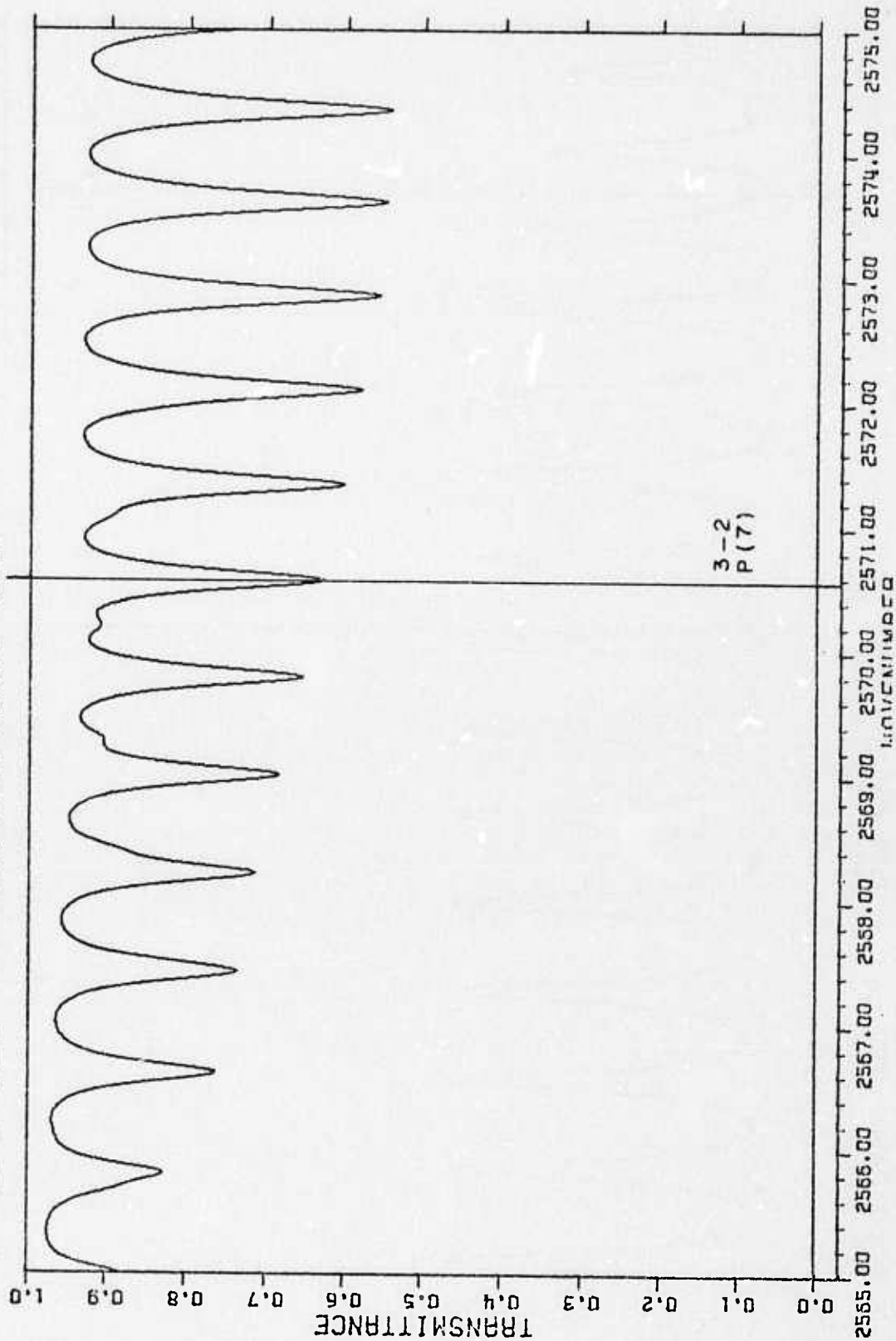


Fig. 24

ABSORBER: N2O  
AMOUNT (TORR): .0020  
TEMP (DEG F): 69.80

06/28/73  
TOTAL PRESSURE (TORR): 760.0  
PATH LENGTH (METER): 1000.

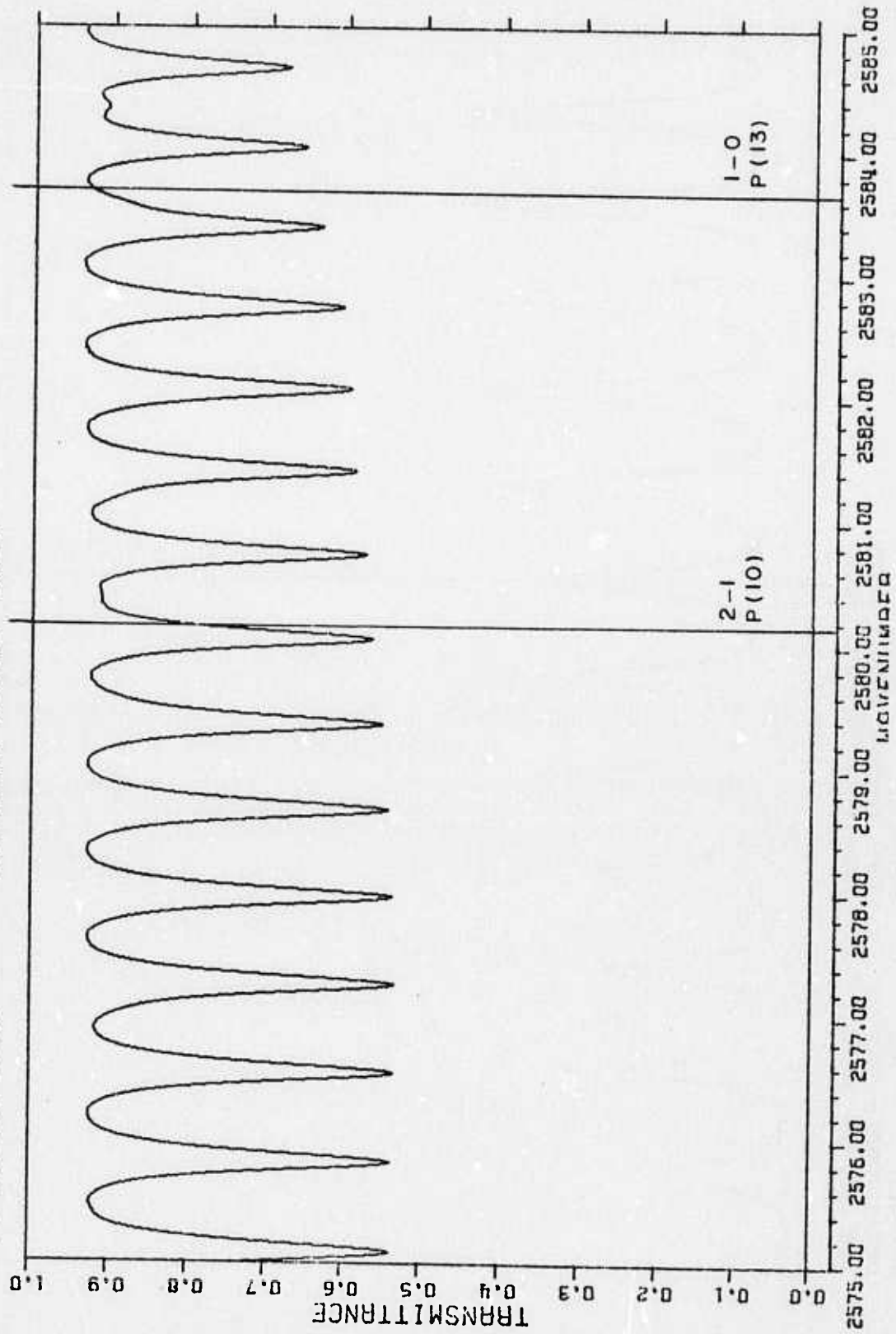


Fig. 25

ABSORBER: N2O  
AMOUNT (TORR): .1000  
TEMP (DEG F): 69.80

06/20/73  
TOTAL PRESSURE (TORR): 760.0  
PATH LENGTH (METER): 1000.

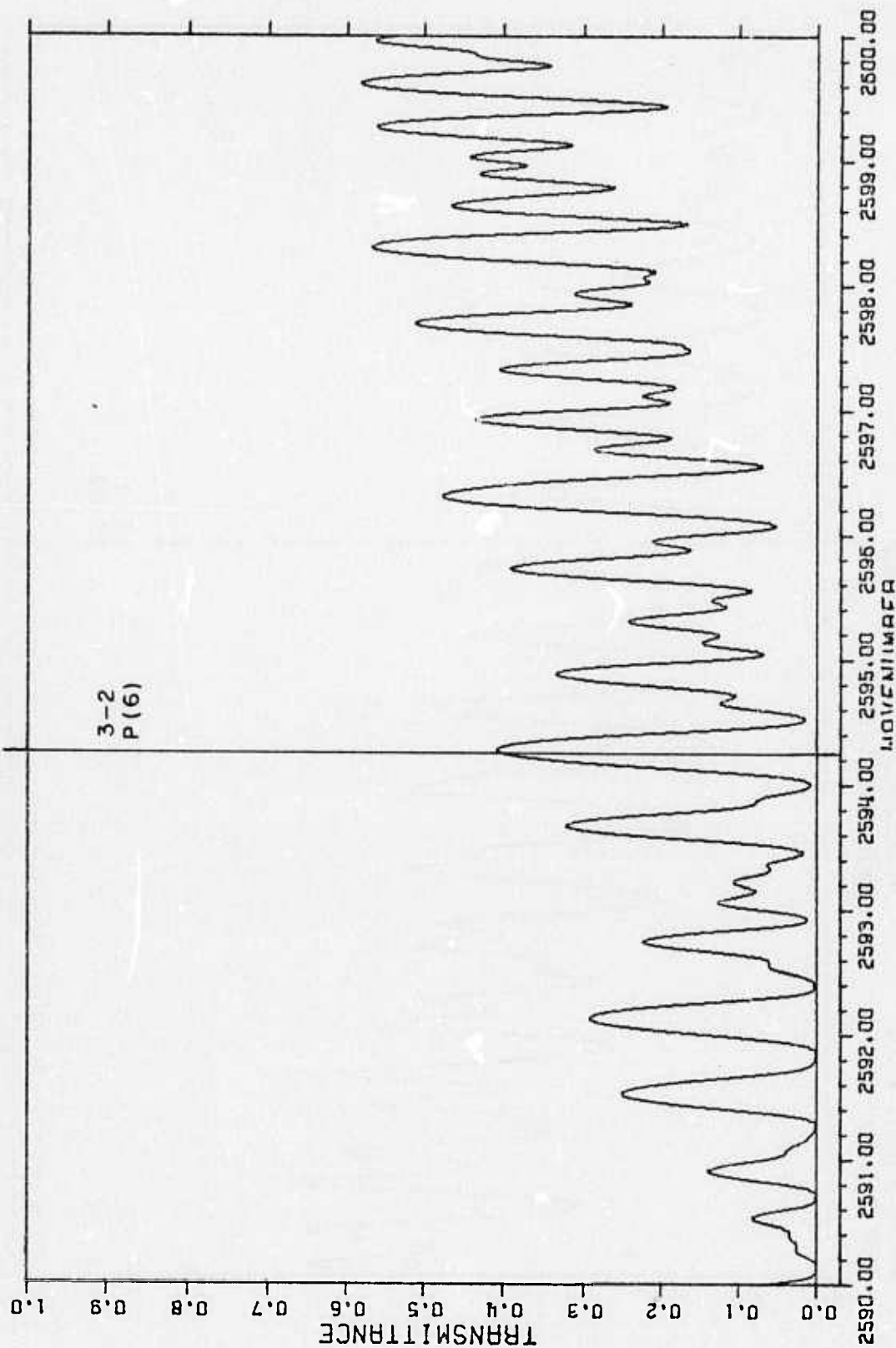


Fig. 26



ABSORBER: N2O  
AMOUNT (TORR): .1000  
TEMP (DEG F): 69.80

06/29/73  
TOTAL PRESSURE (TORR): 760.0  
PATH LENGTH (METER): 1000.

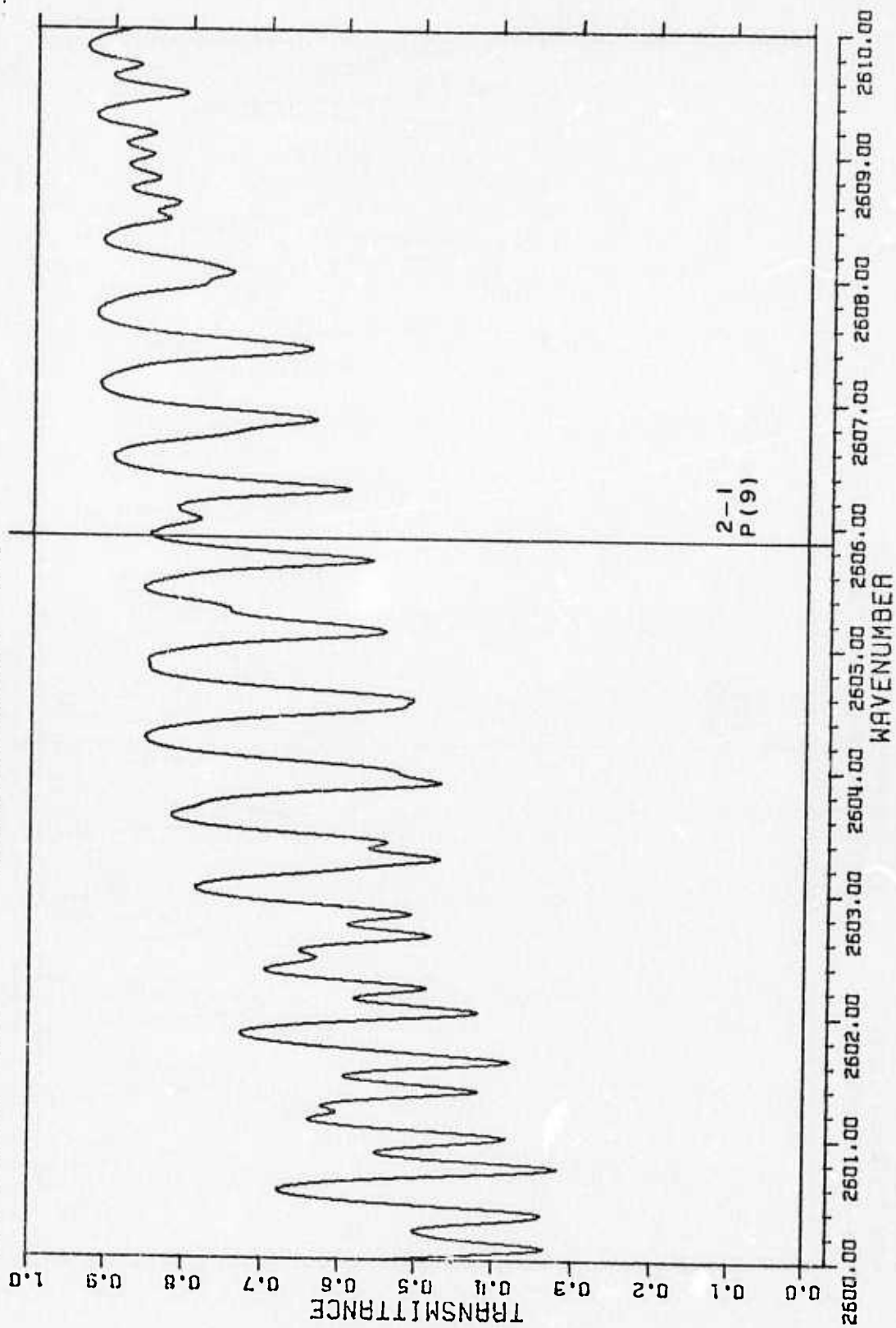


Fig. 27

ABSORBER: N2O  
AMOUNT (TORR): 2.000  
TEMP (DEG F): 69.80

06/29/73  
TOTAL PRESSURE (TORR): 760.0  
PATH LENGTH (METER): 1000.

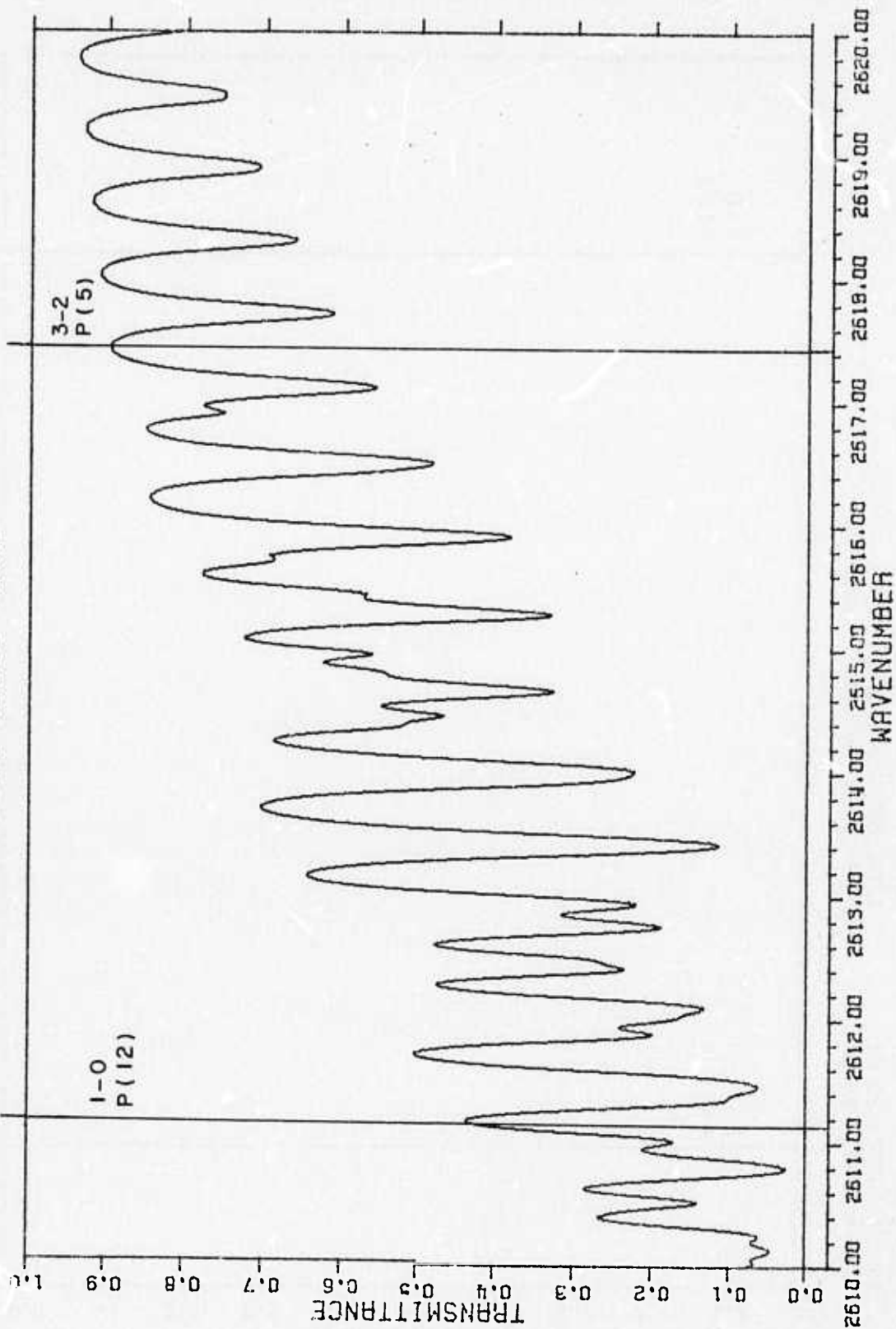


Fig. 28

ABSORBER: N2O  
AMOUNT (TORR): 30.00  
TEMP (DEG F): 69.80

06/29/73  
TOTAL PRESSURE (TORR): 760.0  
PATH LENGTH (METER): 1000.

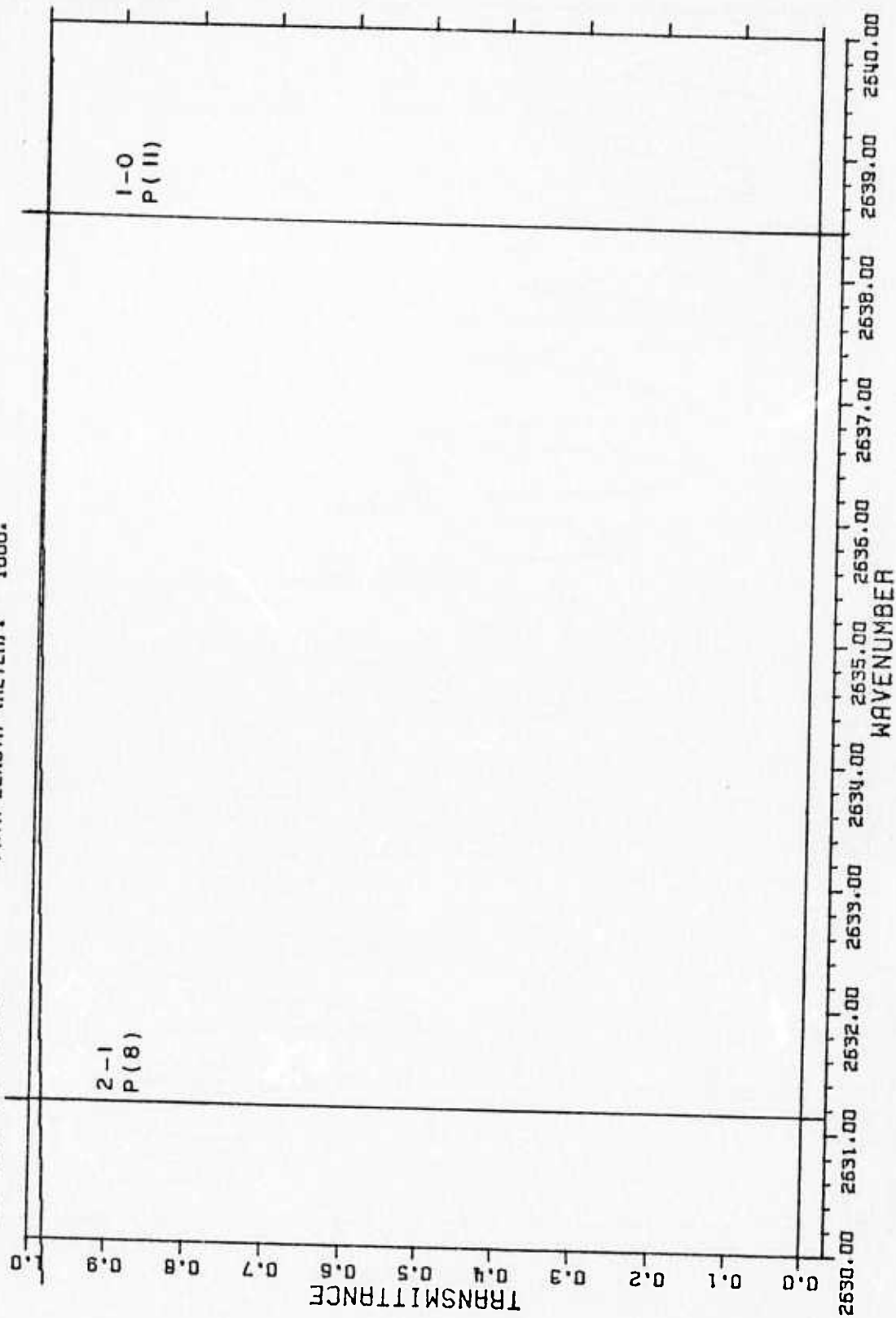


Fig. 29

ABSORBER: N2O  
AMOUNT (TORR): 5.000  
TEMP (DEG F): 59.80

07/11/73  
TOTAL PRESSURE (TORR): 760.0  
PATH LENGTH (METER): 1000.

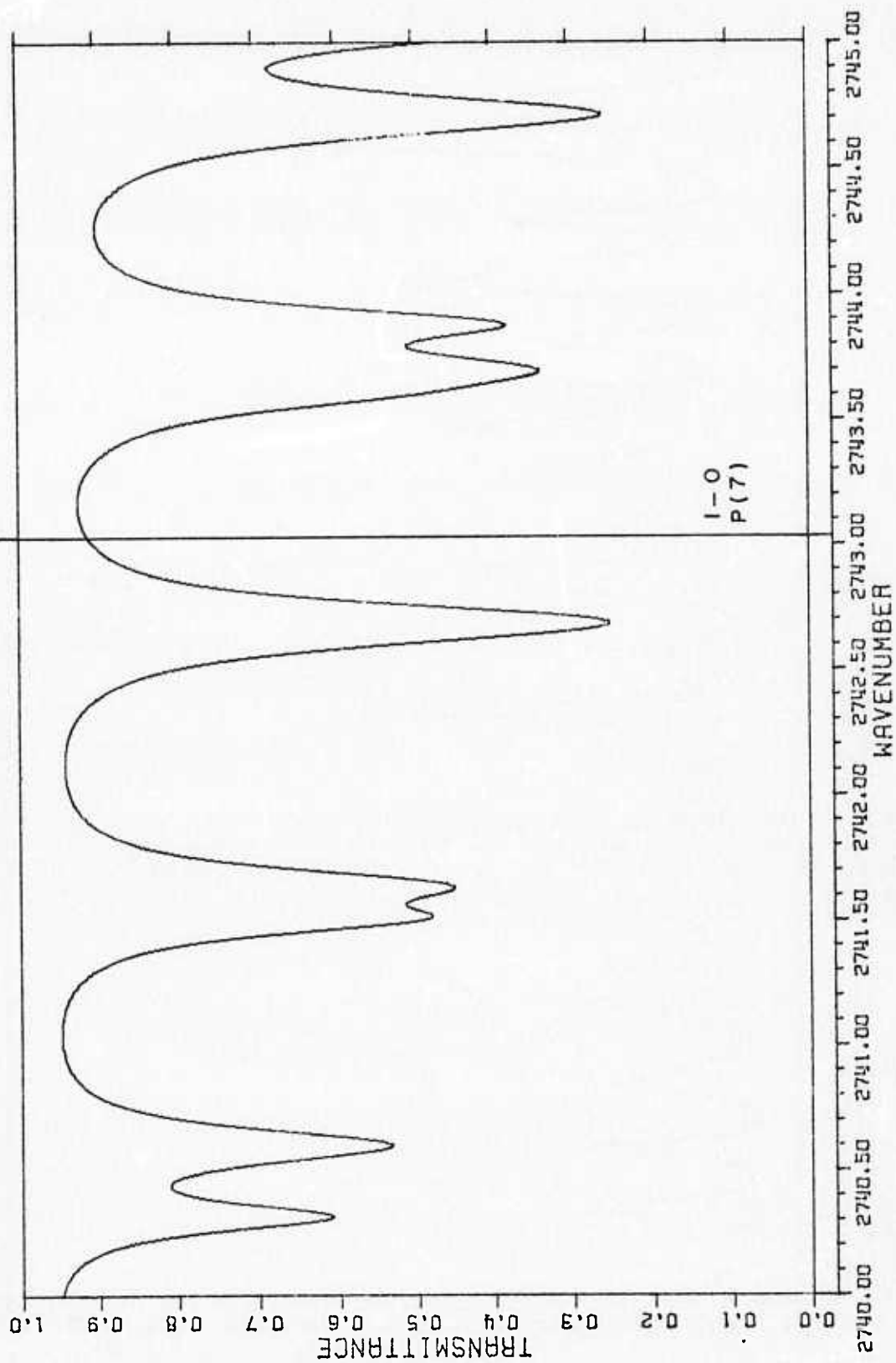


Fig. 30

ABSORBER: N2O  
AMOUNT (TORR): 1.000  
TEMP (DEG F): 69.80

06/28/73  
TOTAL PRESSURE (TORR): 760.0  
PATH LENGTH (METER): 1000.

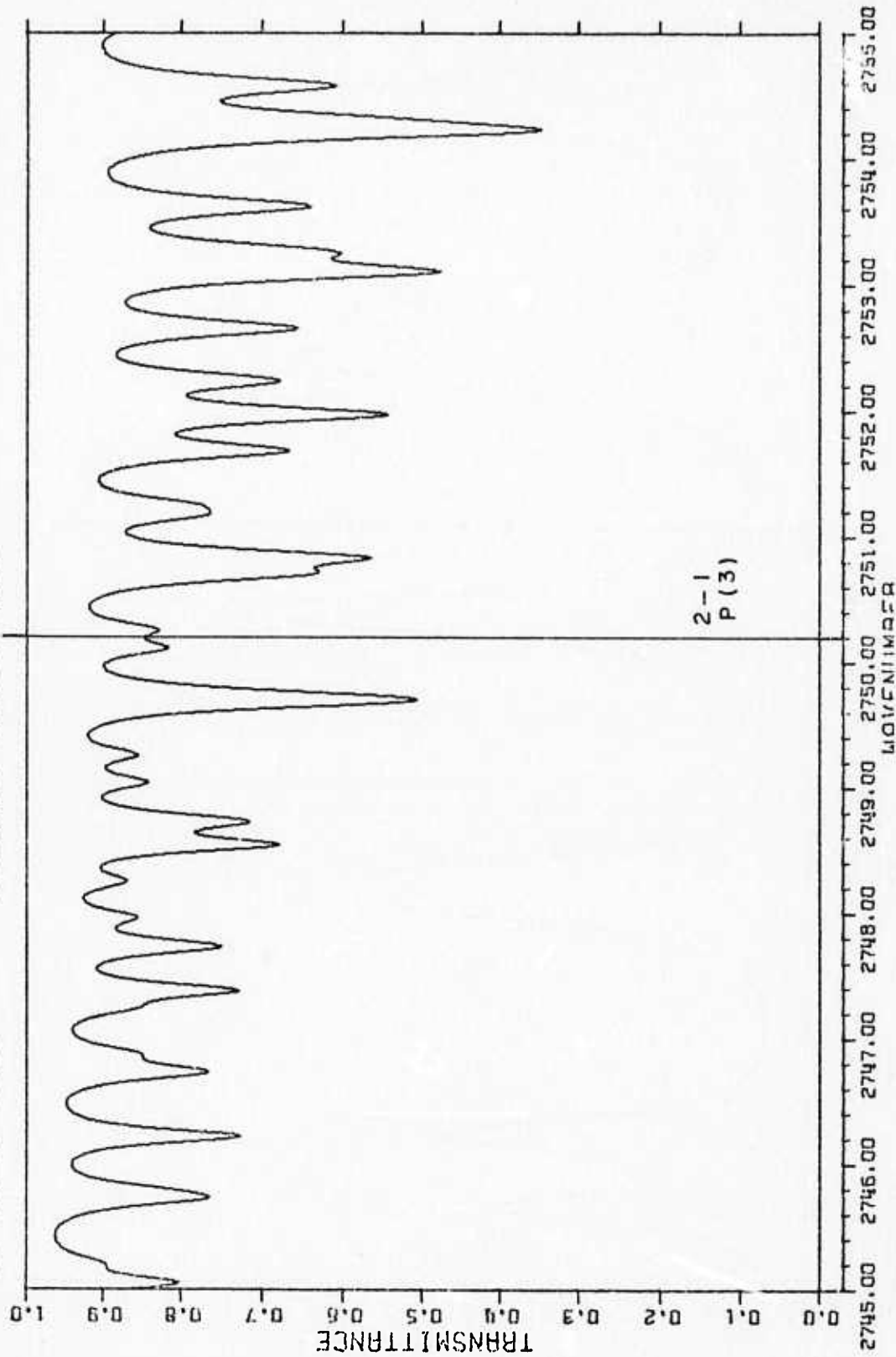


Fig. 31

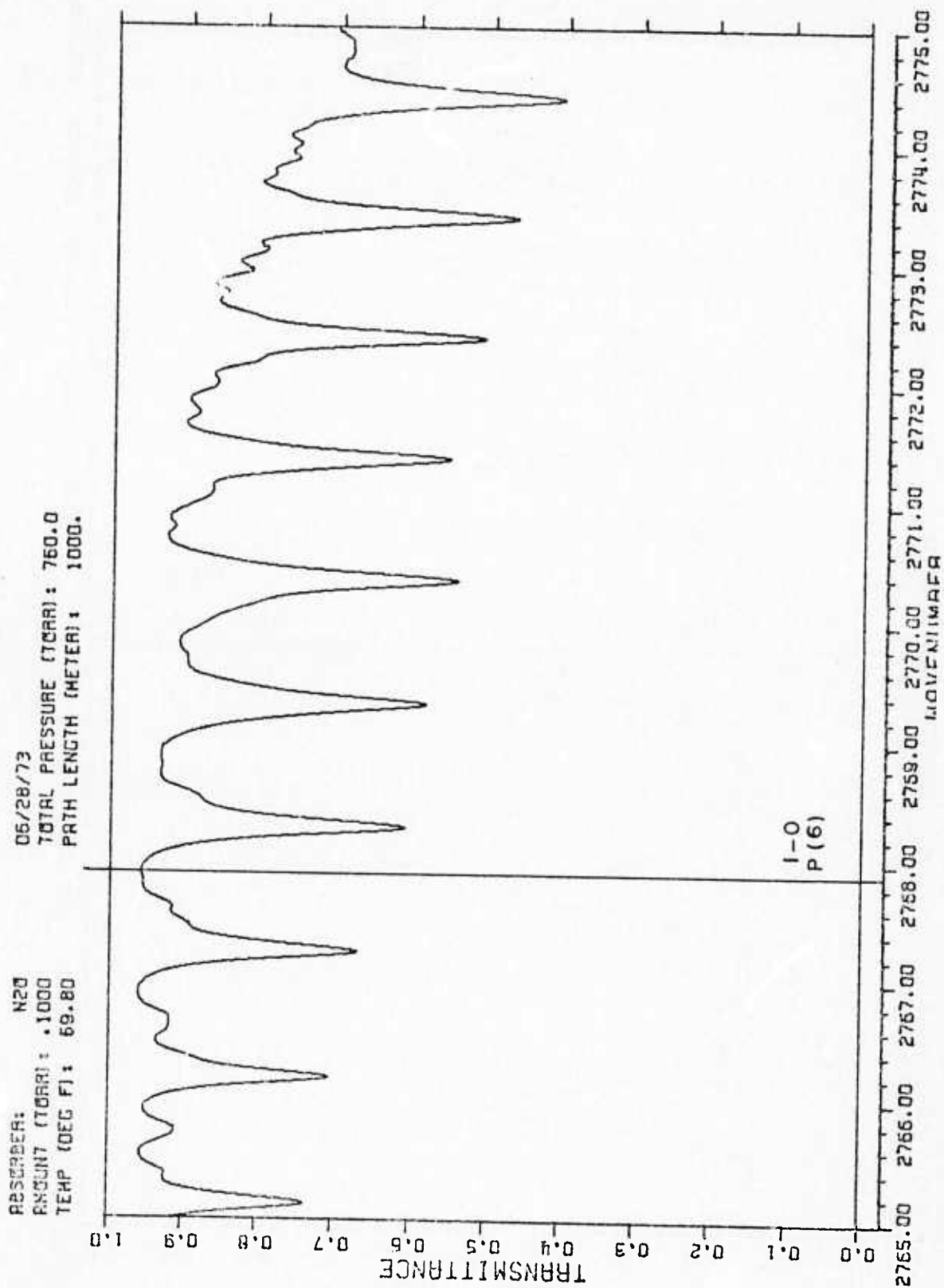


Fig. 32



ABSORBER: N2O  
AMOUNT (TORR): .1000  
TEMP (DEG F): 69.80

07/13/73  
TOTAL PRESSURE (TORR): 760.0  
PATH LENGTH (METER): 1000.

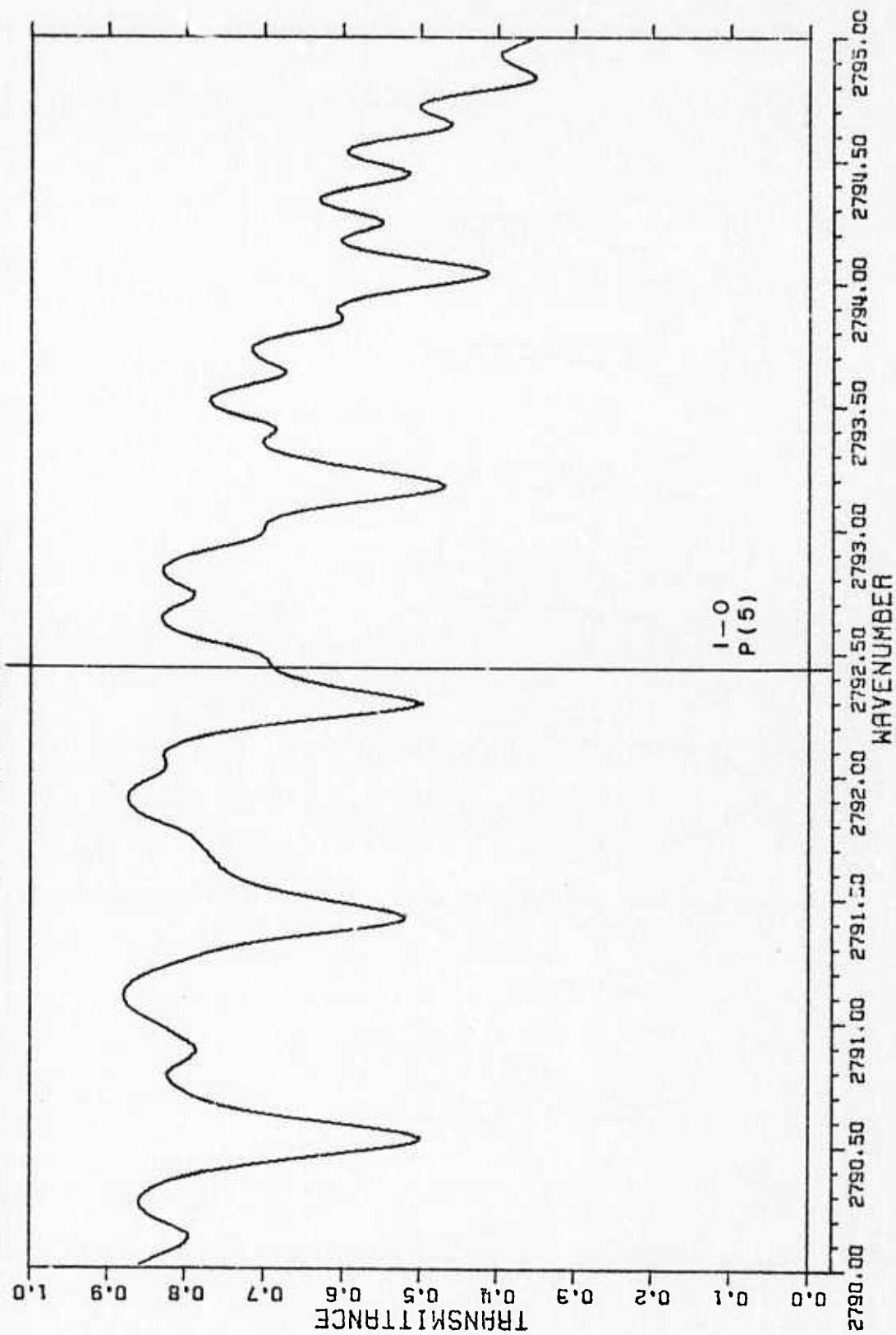


Fig. 33

ABSORBER: N2O  
AMOUNT (MG/CM): 1.000  
TEMP (DEG F): 69.80

07/13/73  
TOTAL PRESSURE (TORR): 760.0  
PATH LENGTH (METER): 1000.

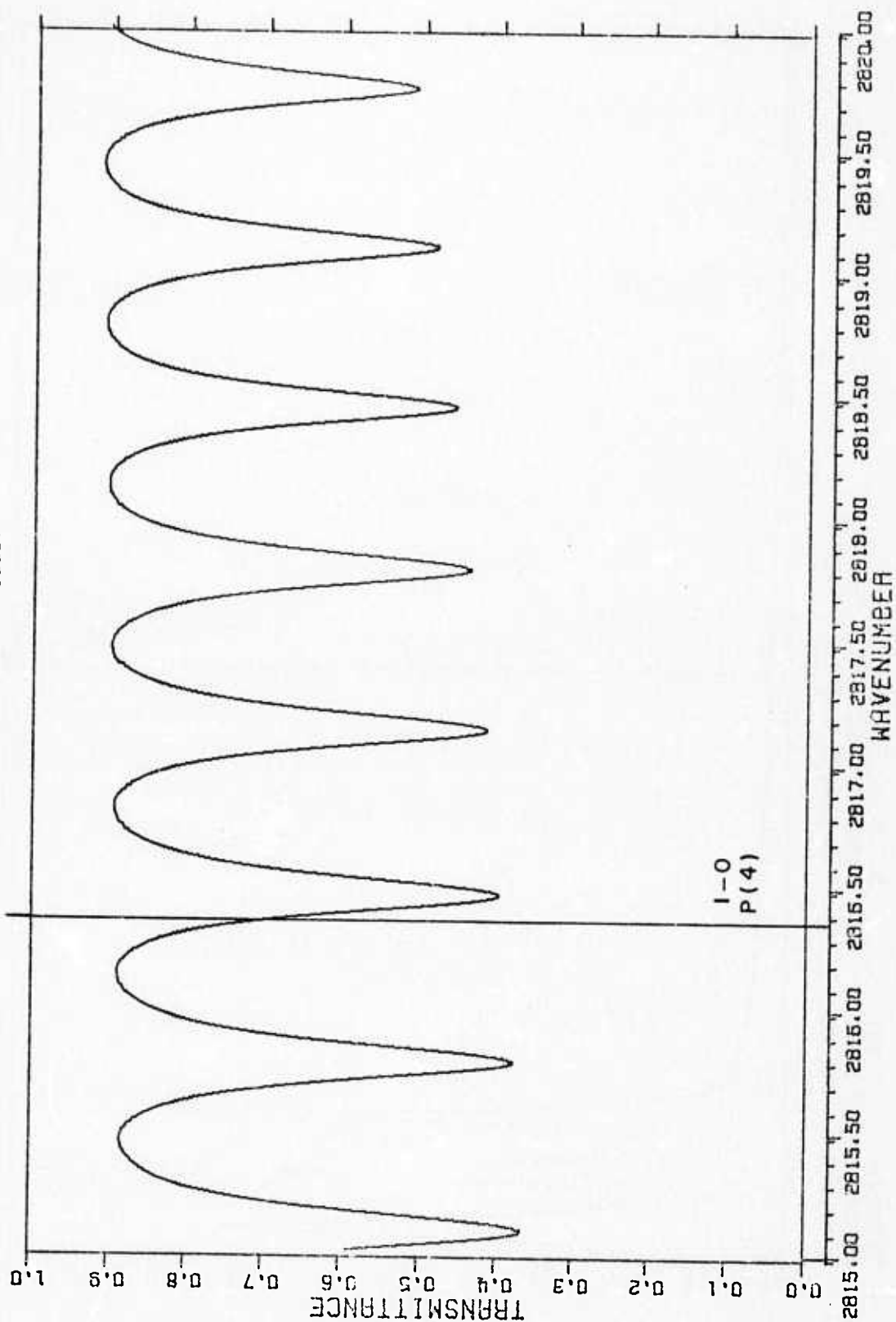


Fig. 34

ABSORBER: N2D  
AMOUNT (TERR): 10.00  
TEMP (DEG F): 69.80

07/18/73  
TOTAL PRESSURE (TERR): 760.0  
PATH LENGTH (METER): 1000.

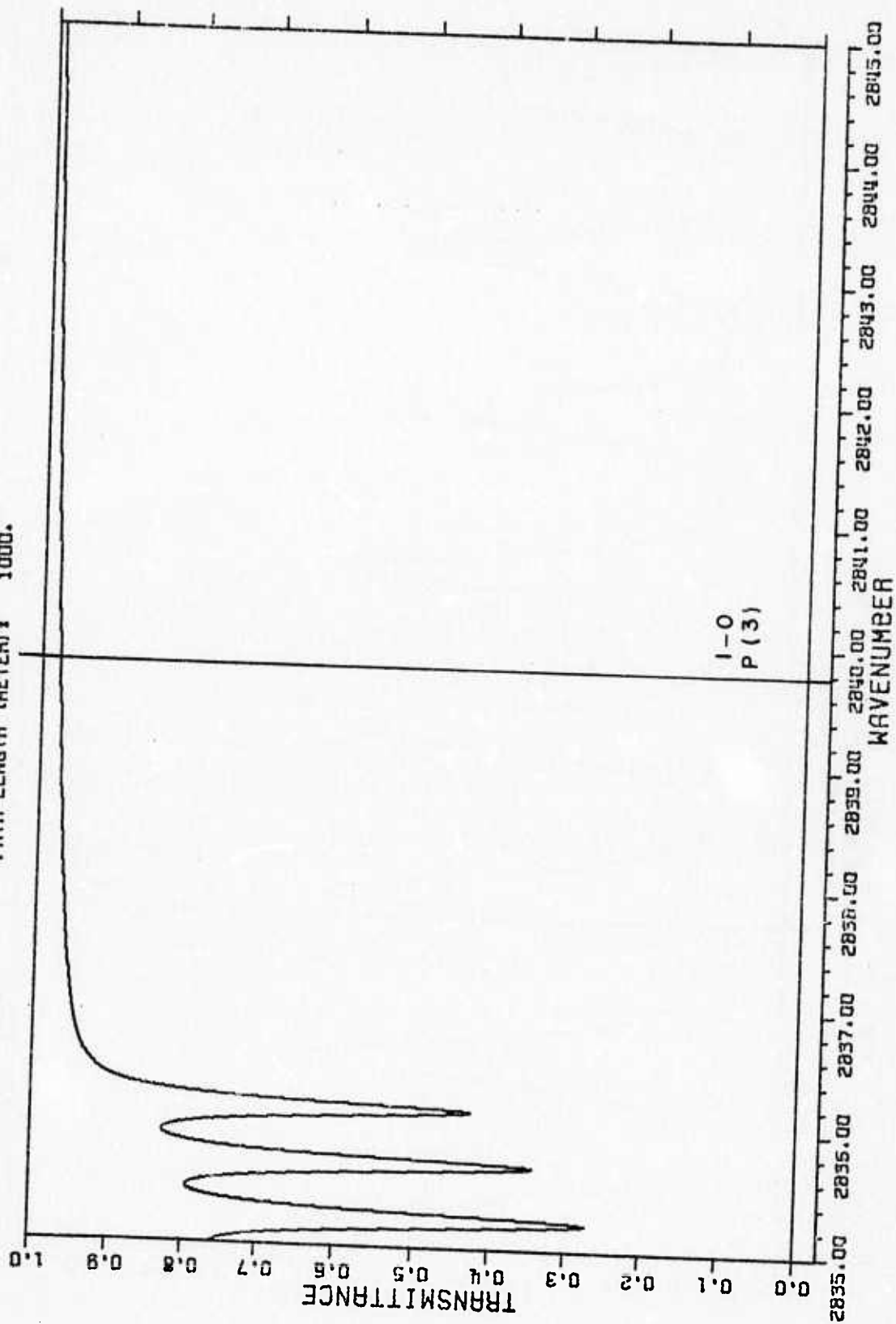


Fig. 35

ABSORBER: M20  
AMOUNT (TORR): 15.00  
TEMP (DEG F): 69.80

07/17/73  
TOTAL PRESSURE (TORR): 760.0  
PATH LENGTH (METER): 10000

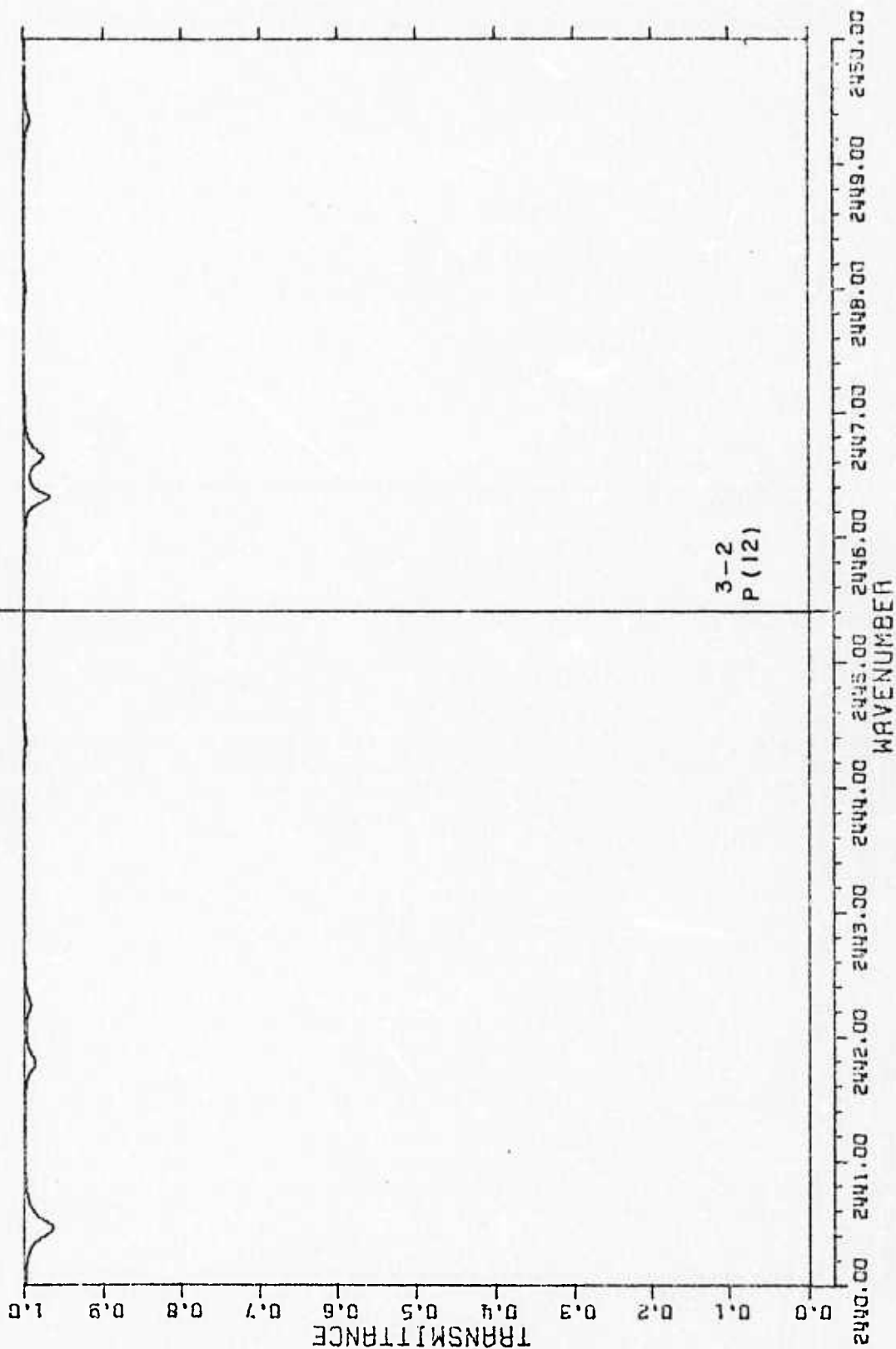


Fig. 36

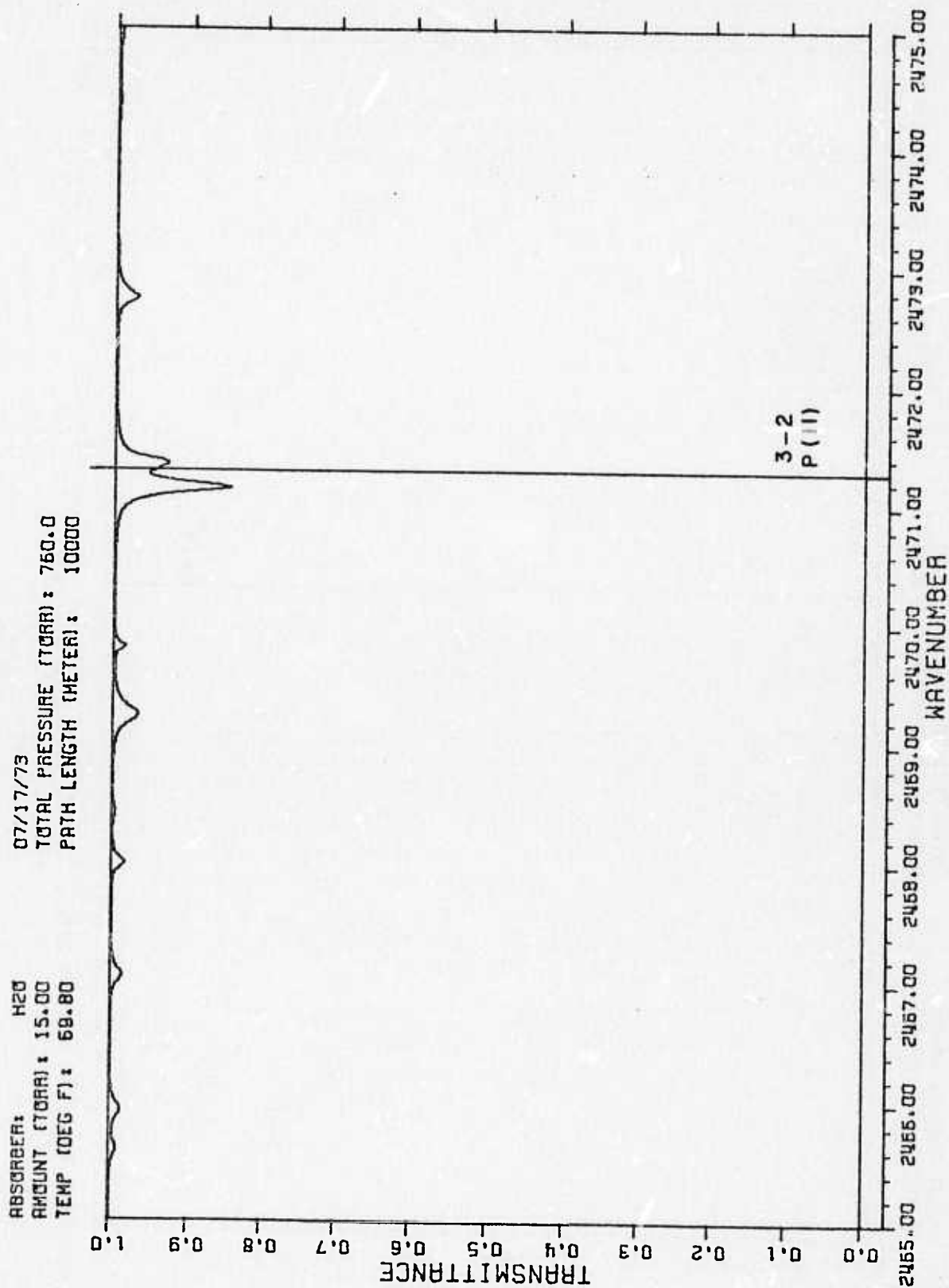


Fig. 37

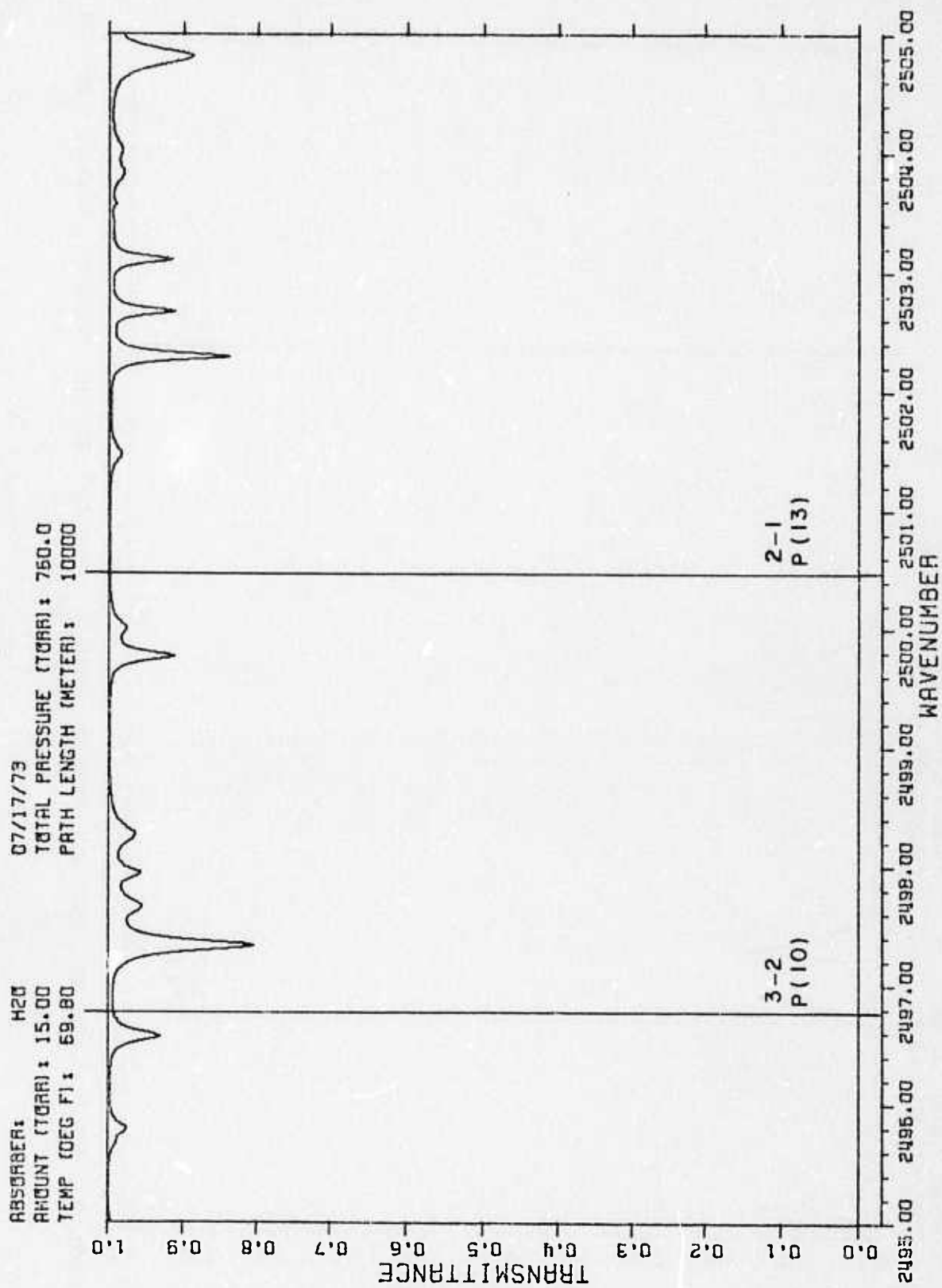


Fig. 38



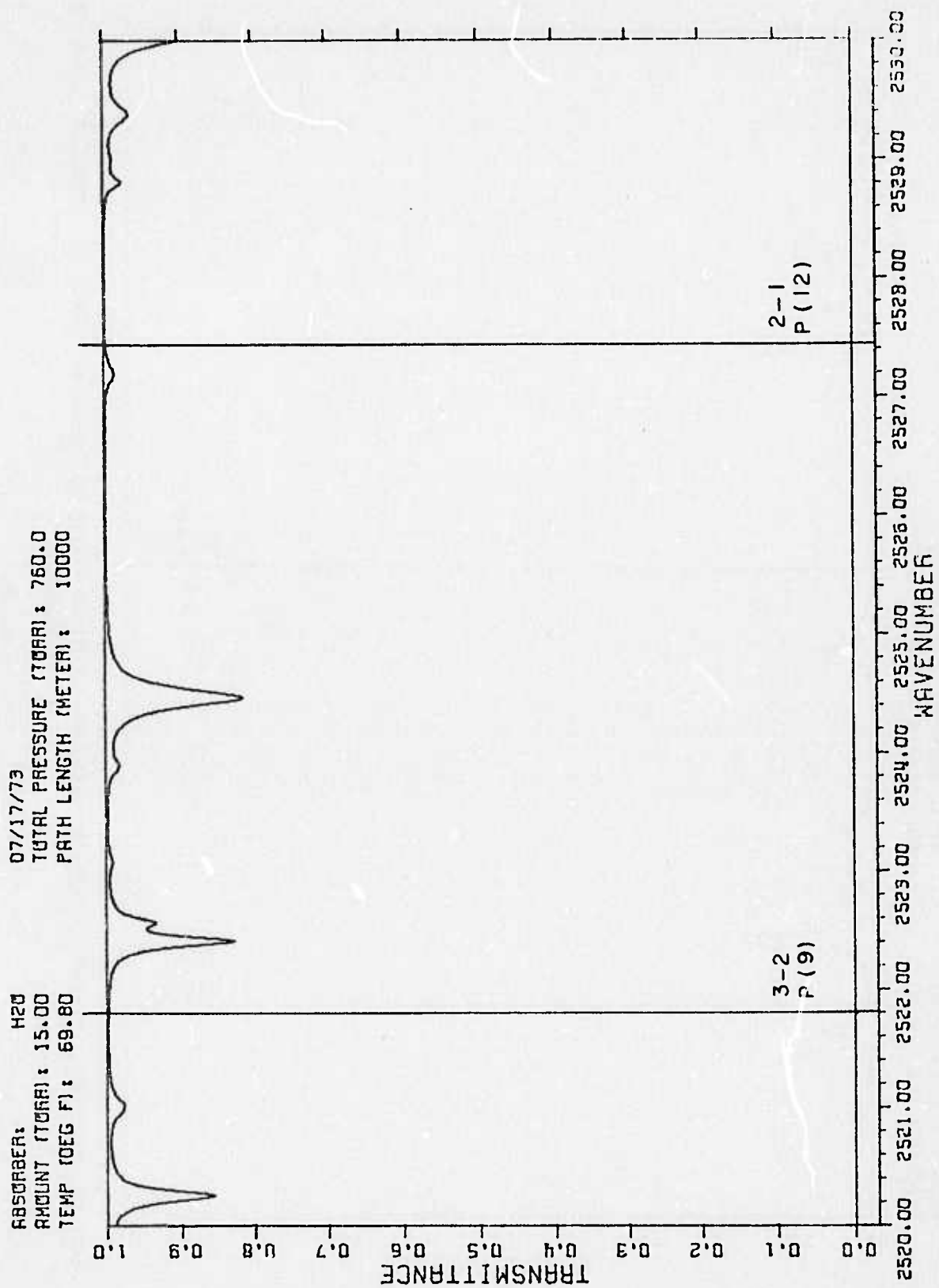


Fig. 39

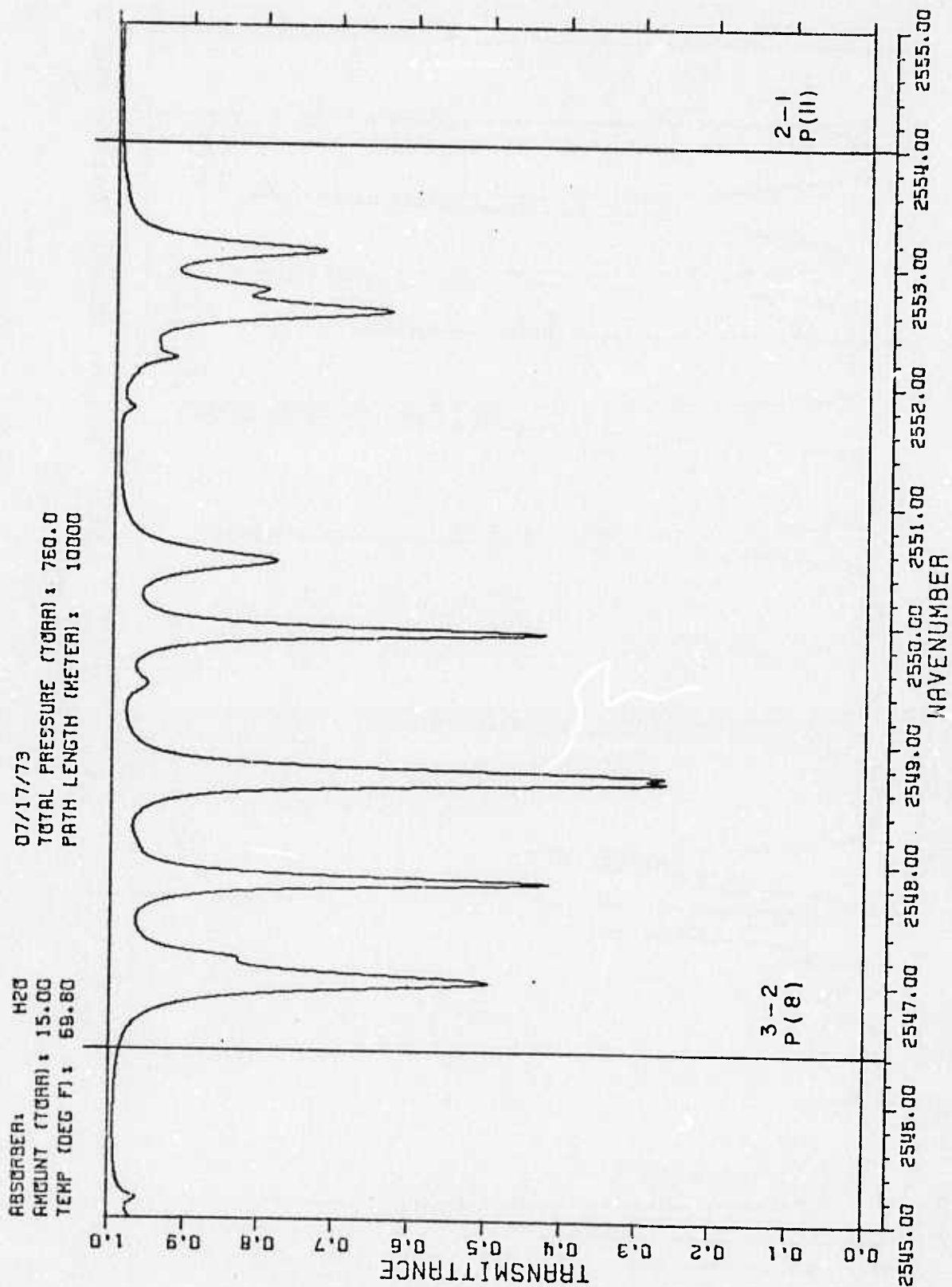


Fig. 40

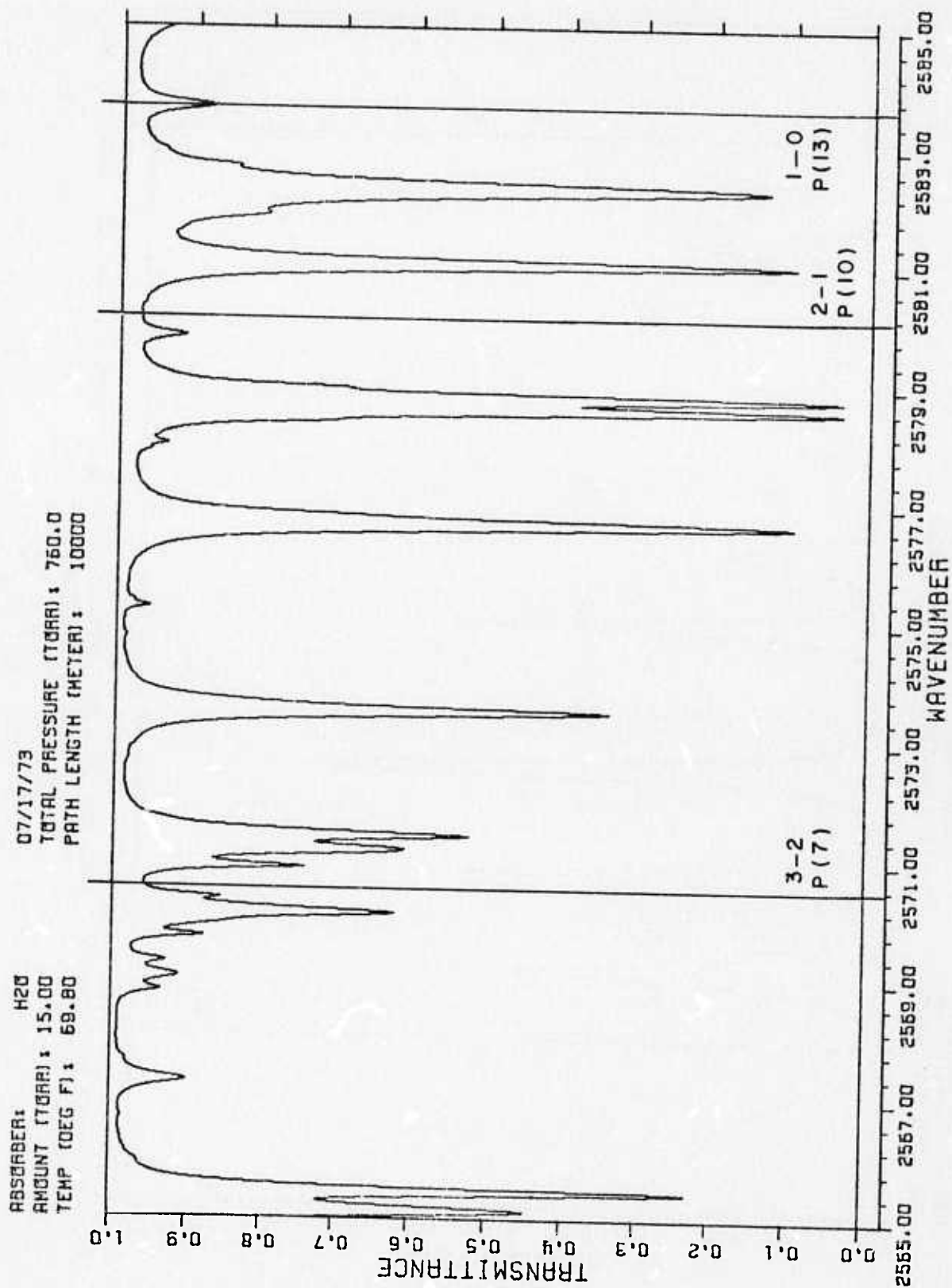


Fig. 41

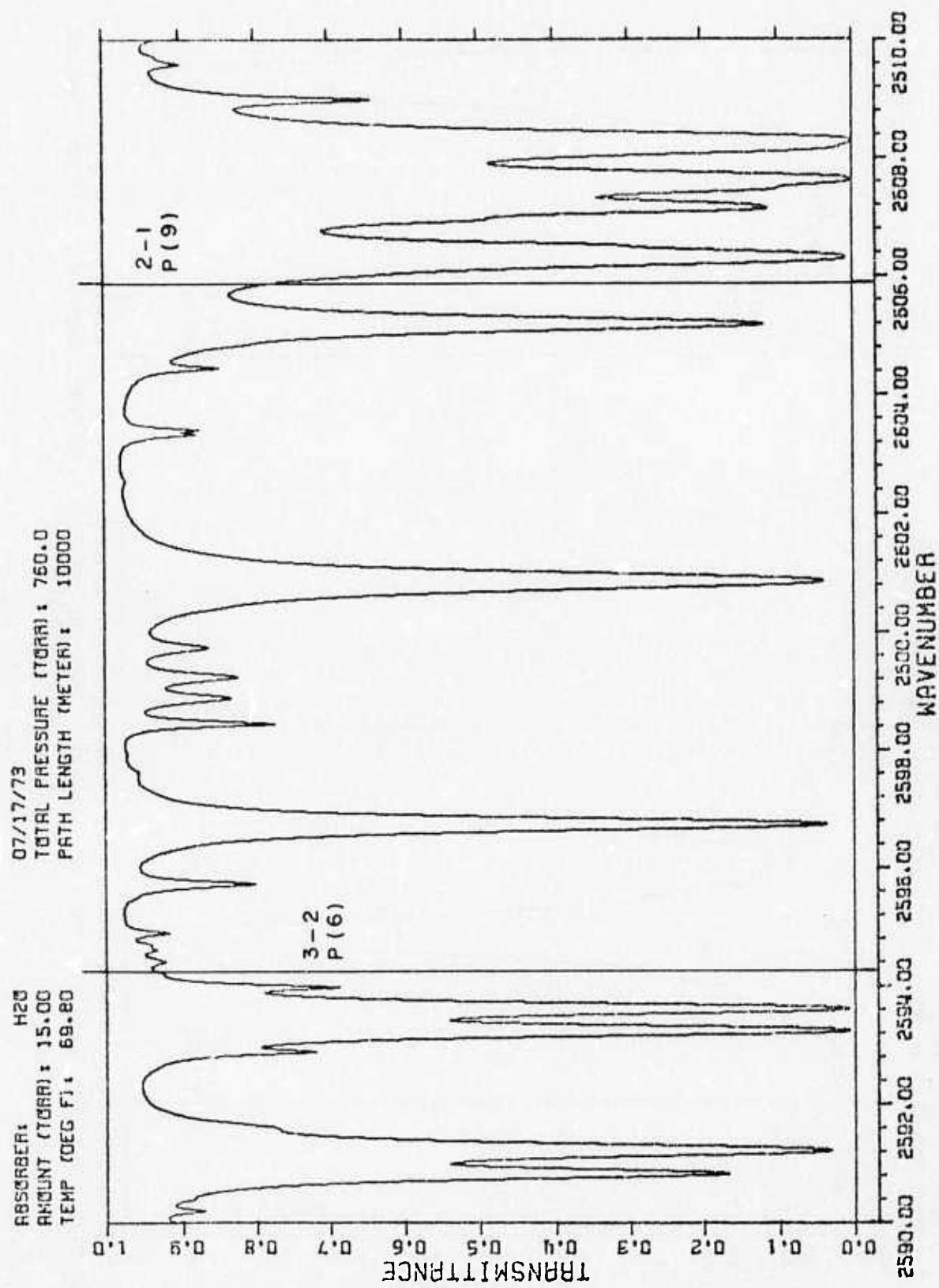


Fig. 42

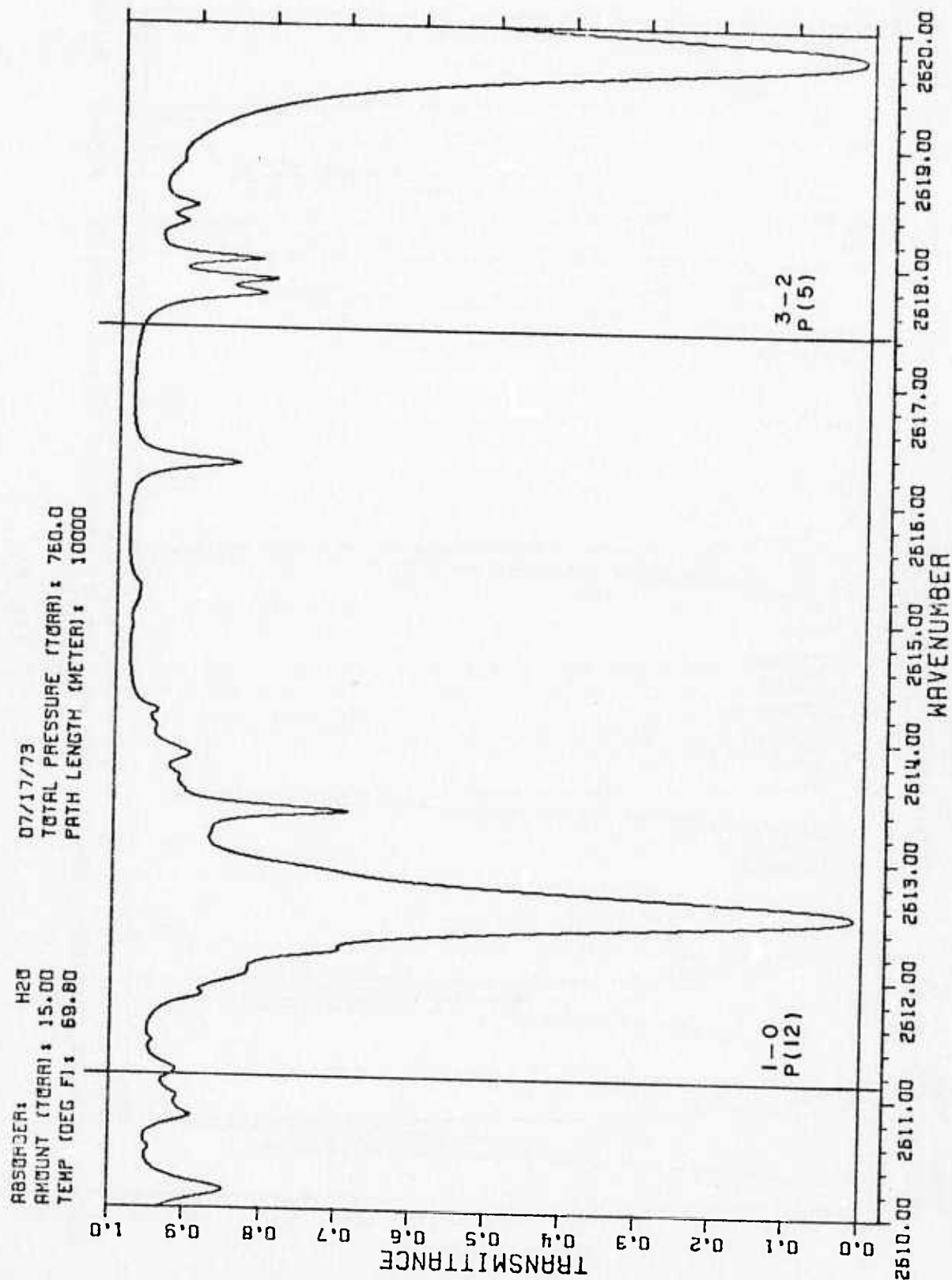


Fig. 43

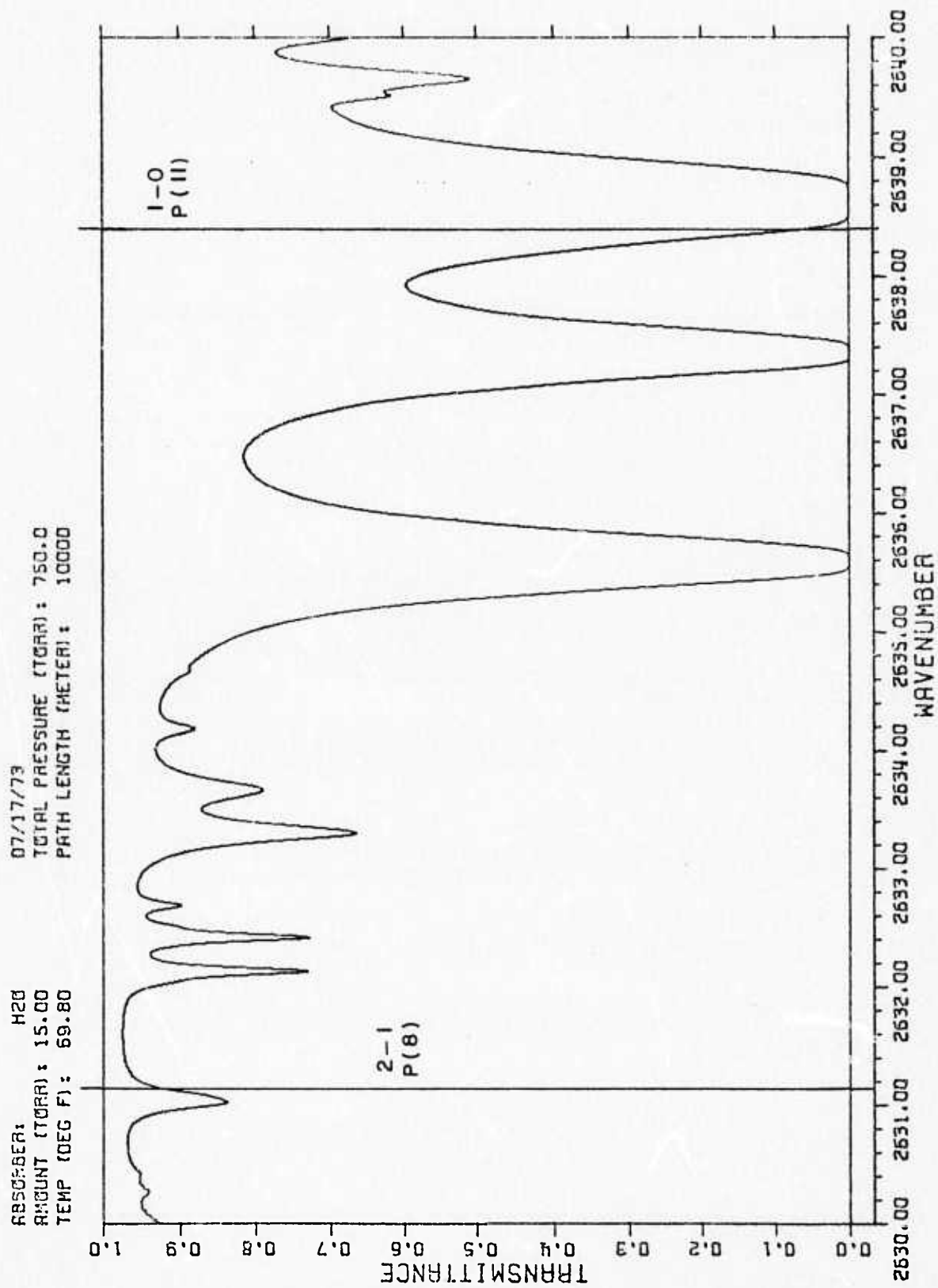


Fig. 44



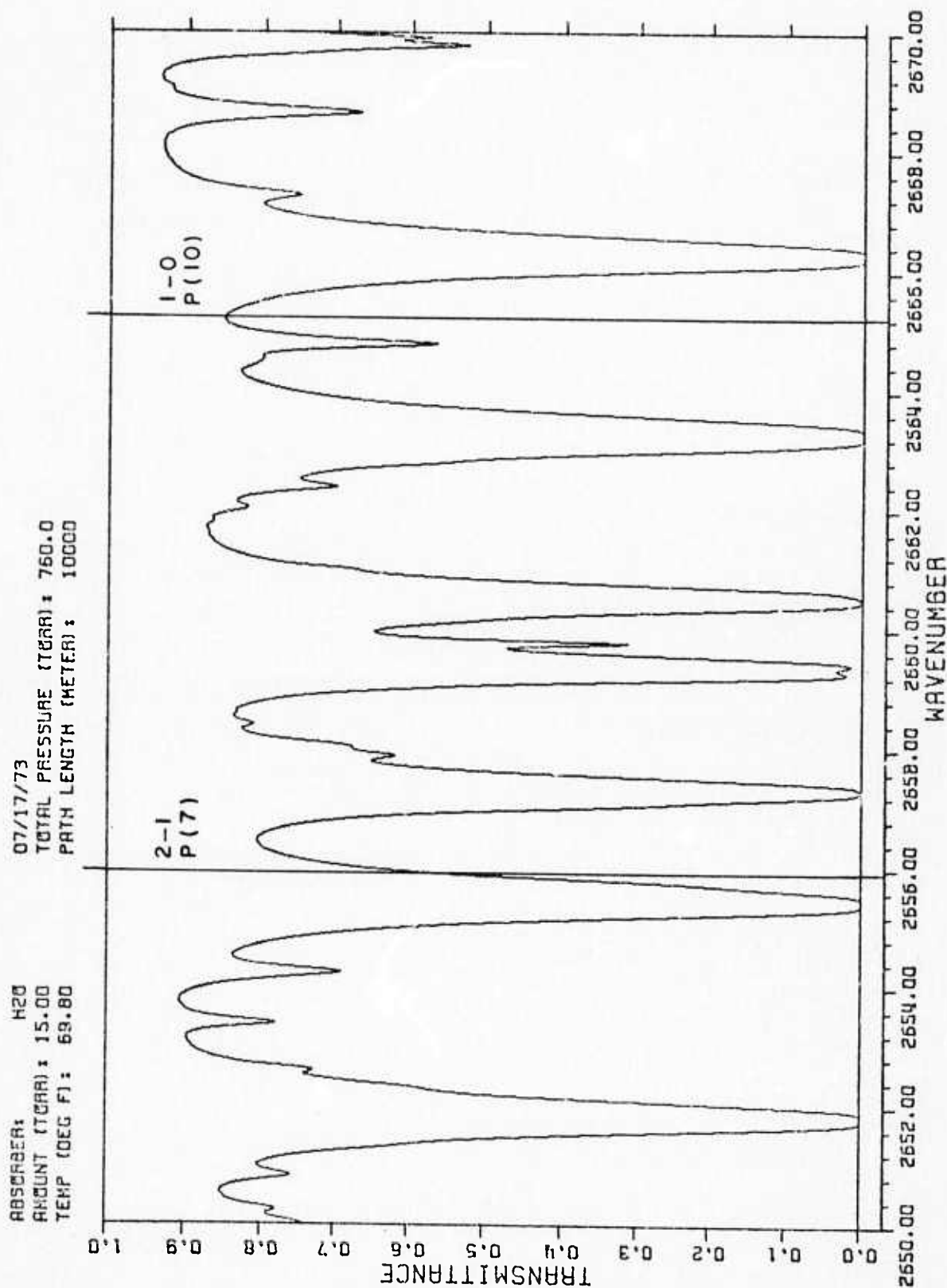


Fig. 45

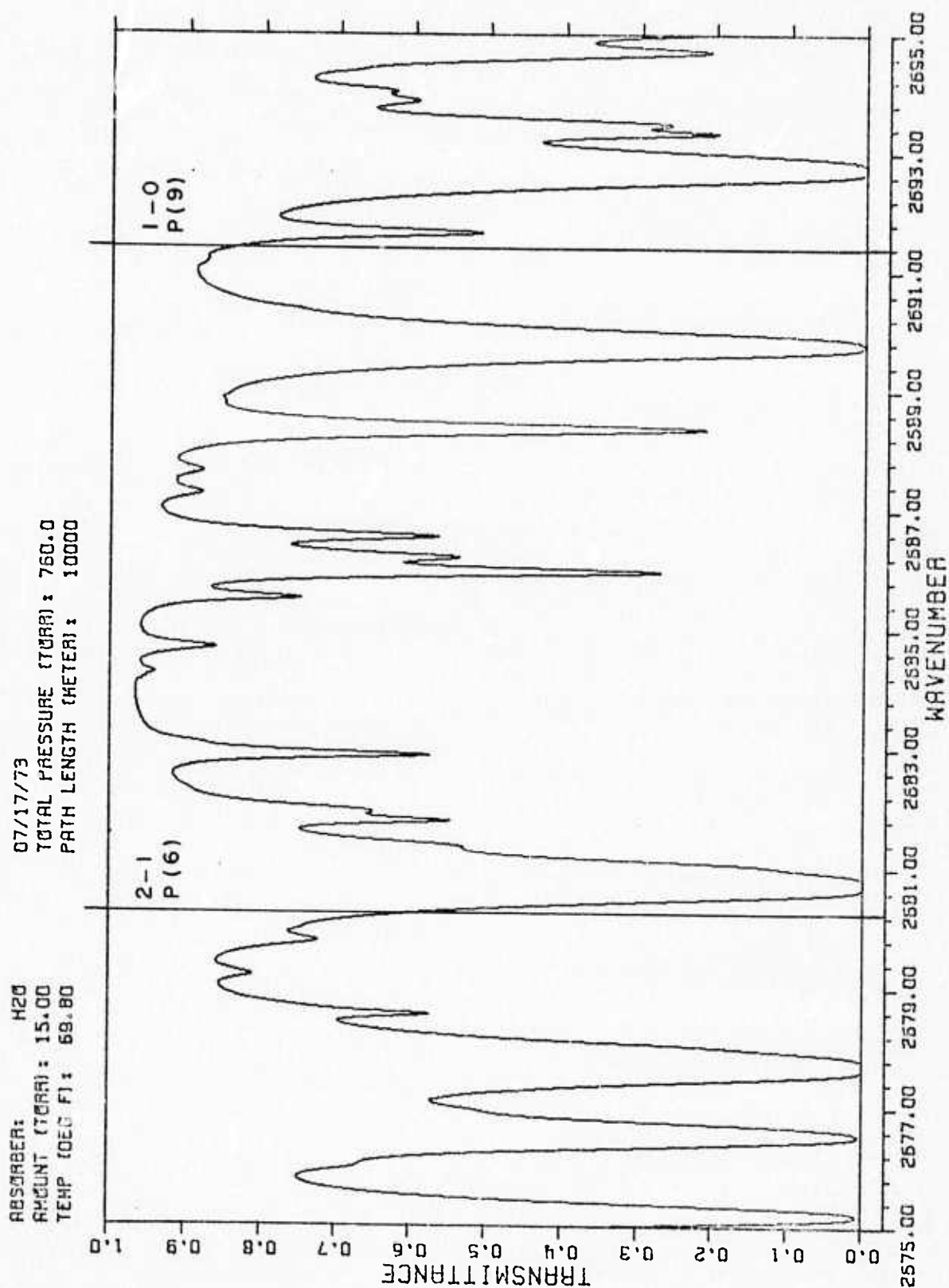


Fig. 46

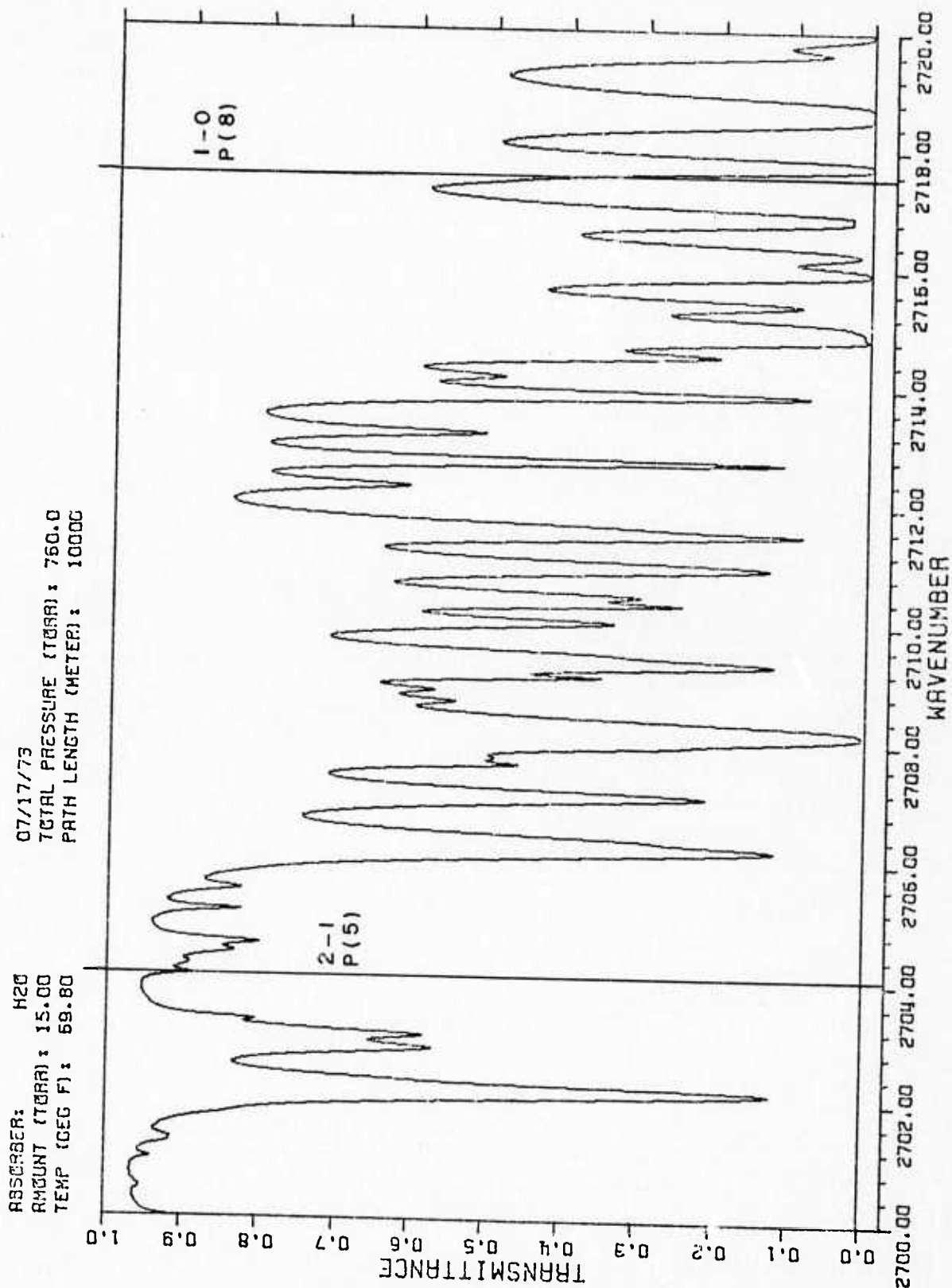


Fig. 47

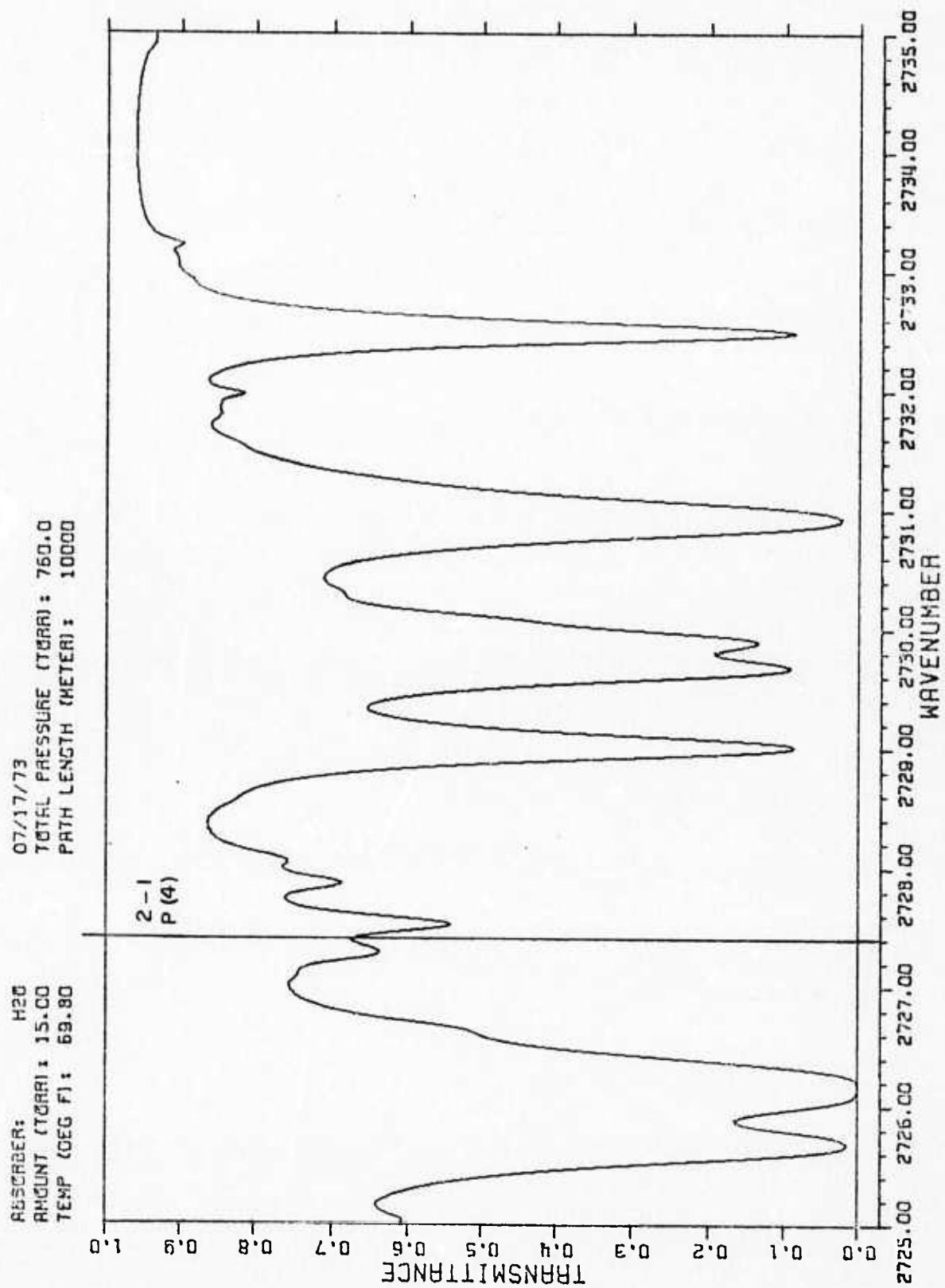


Fig. 48

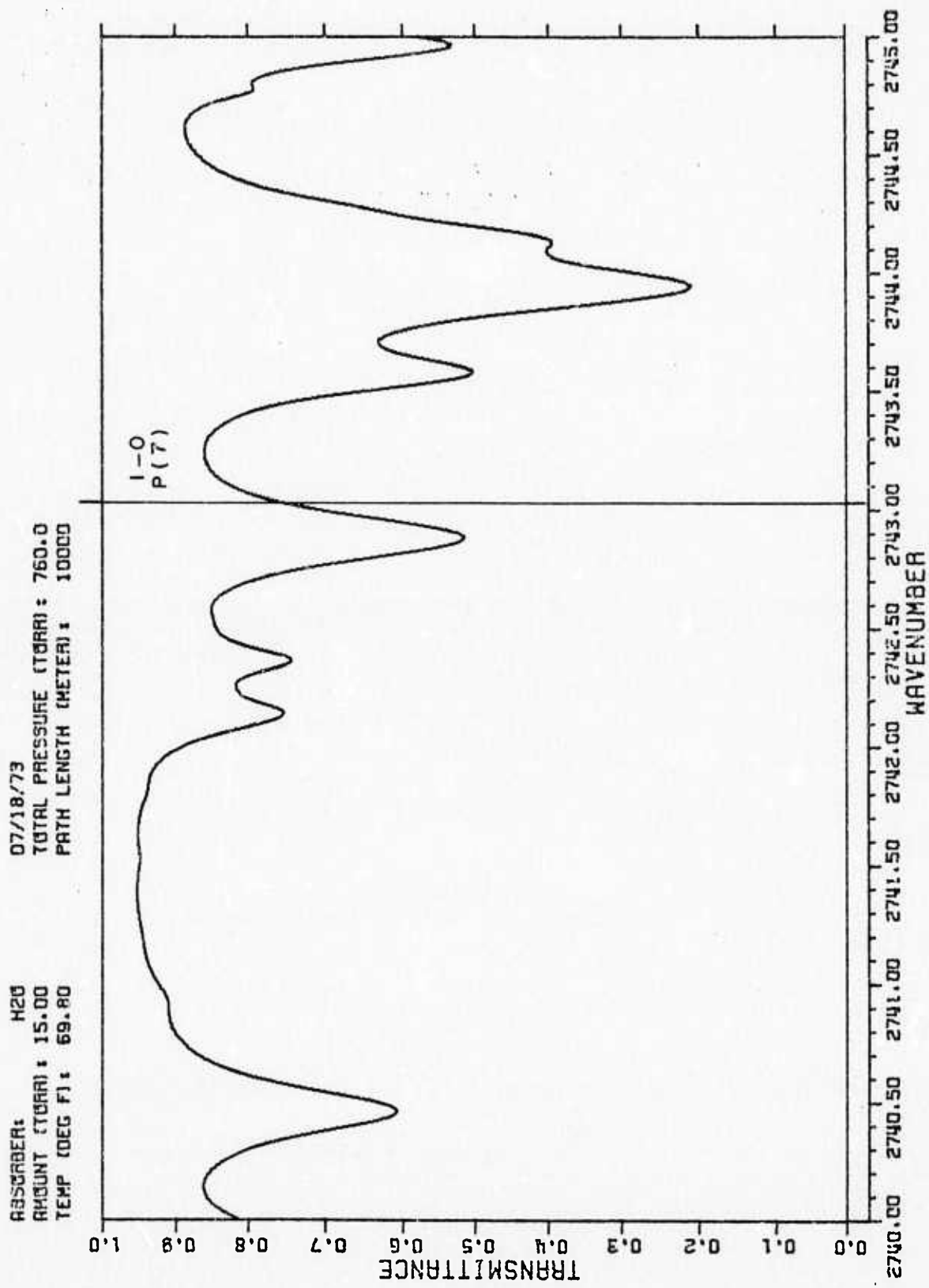


Fig. 49

07/17/73  
TOTAL PRESSURE (TORR): 750.0  
PATH LENGTH (METER): 10000

ABSORBER: H<sub>2</sub>O  
AMOUNT (TORR): 15.00  
TEMP (DEG F): 69.80

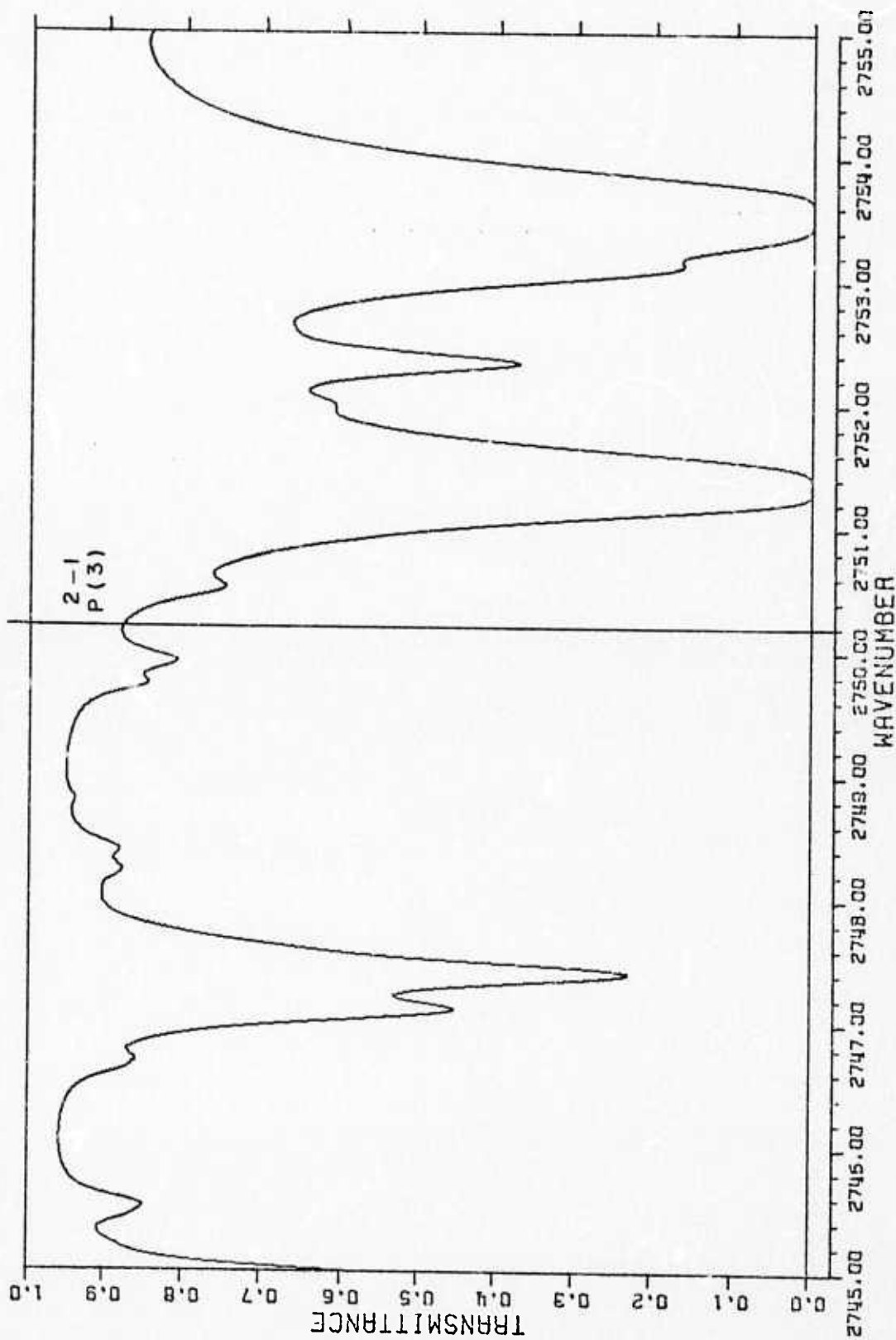


Fig. 50



ABSORBER: H2O  
AMOUNT (TCRR): 15.00  
TEMP (DEG F): 69.80

07/17/73  
TOTAL PRESSURE (TCRR): 760.0  
PATH LENGTH (METER): 10000

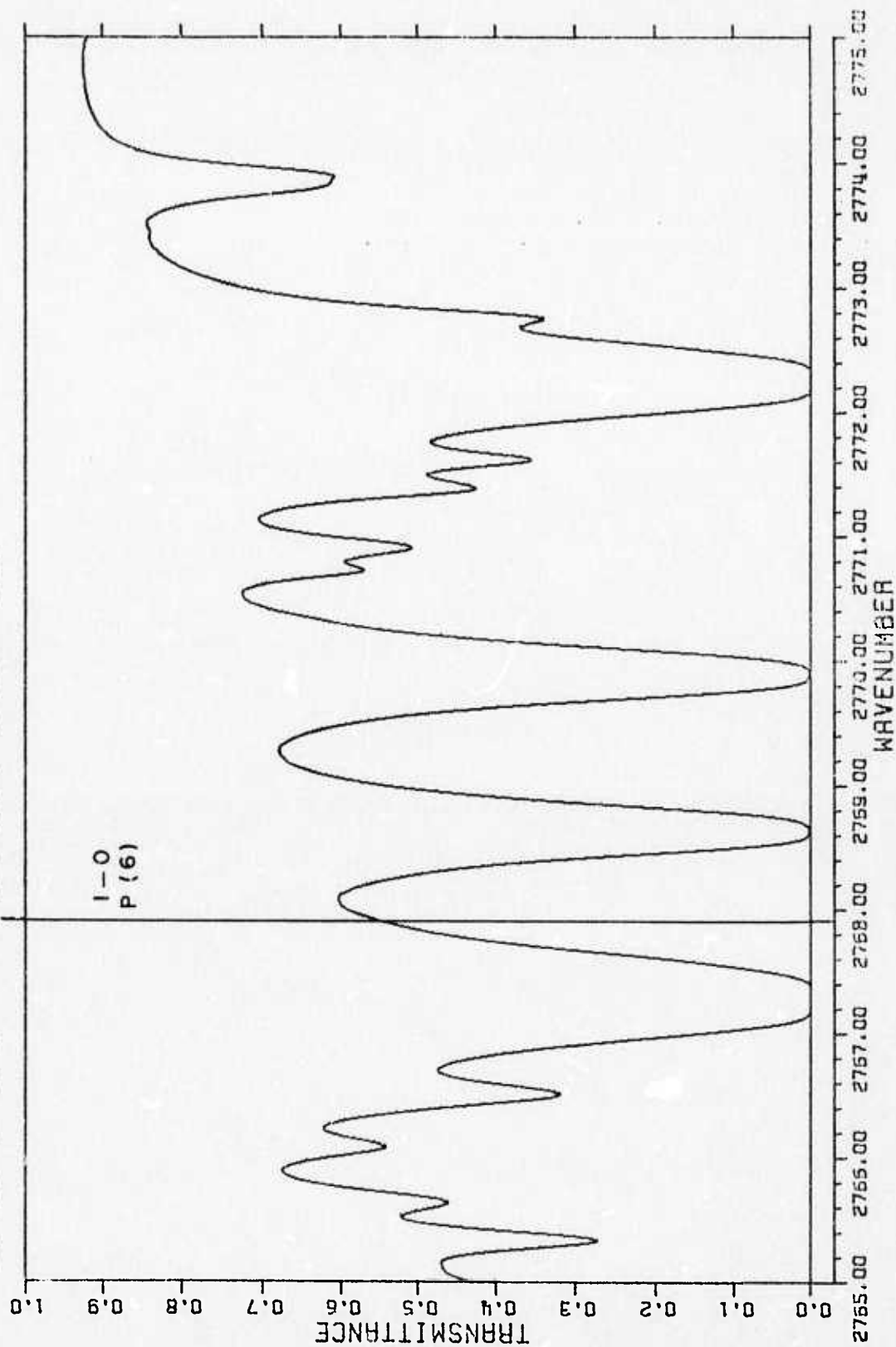


Fig. 51

ABSORBER: H<sub>2</sub>O  
AMOUNT (TORR): 15.00  
TEMP (DEC F): 69.80

07/17/73  
TOTAL PRESSURE (TORR): 760.0  
PATH LENGTH (METER): 10000

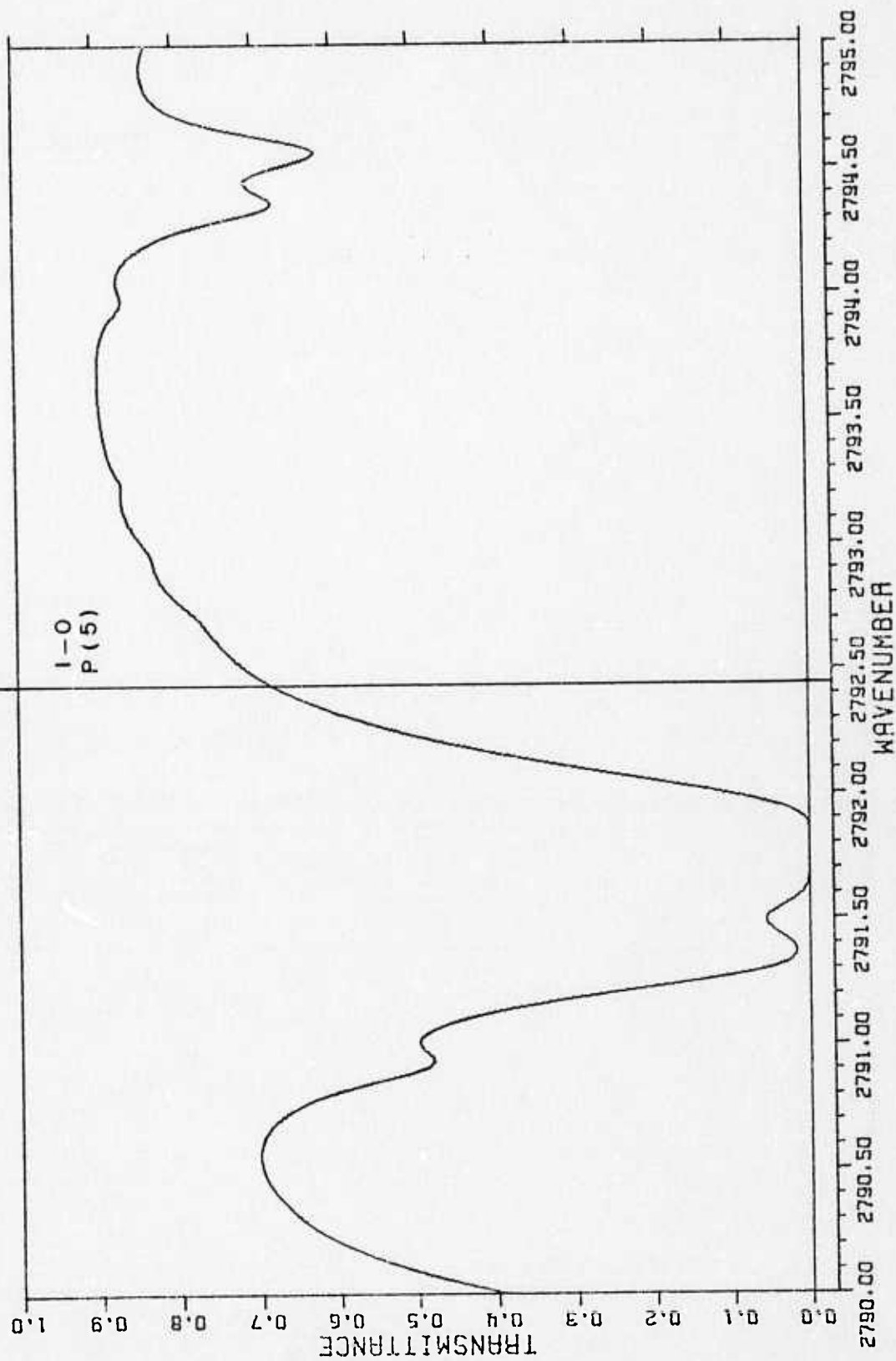


Fig. 52

ABSORBER: H<sub>2</sub>O  
AMOUNT (TORR): 15.00  
TEMP (DEG F): 69.80

07/17/73

TOTAL PRESSURE (TORR): 760.0  
PATH LENGTH (METER): 10000

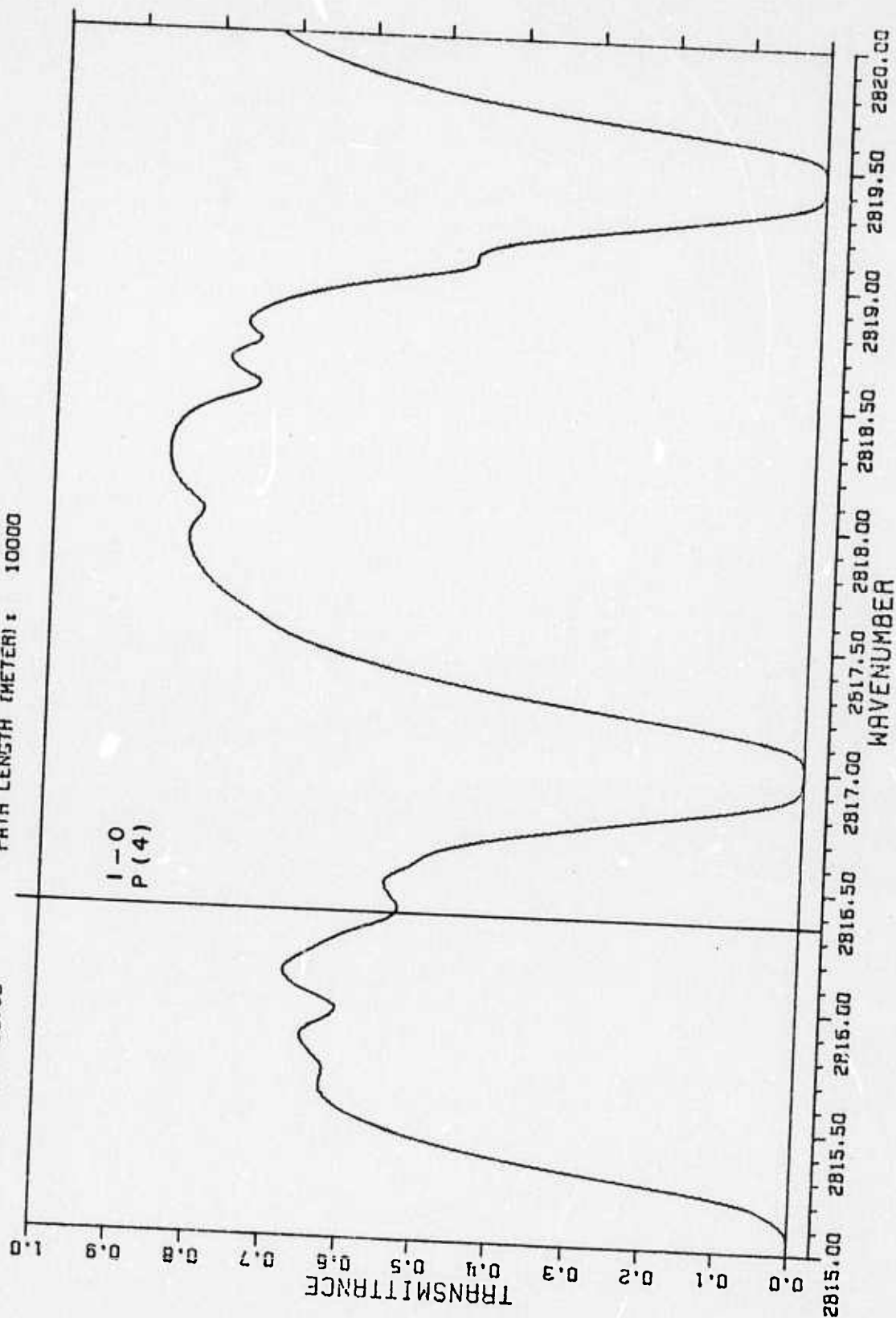


Fig. 53

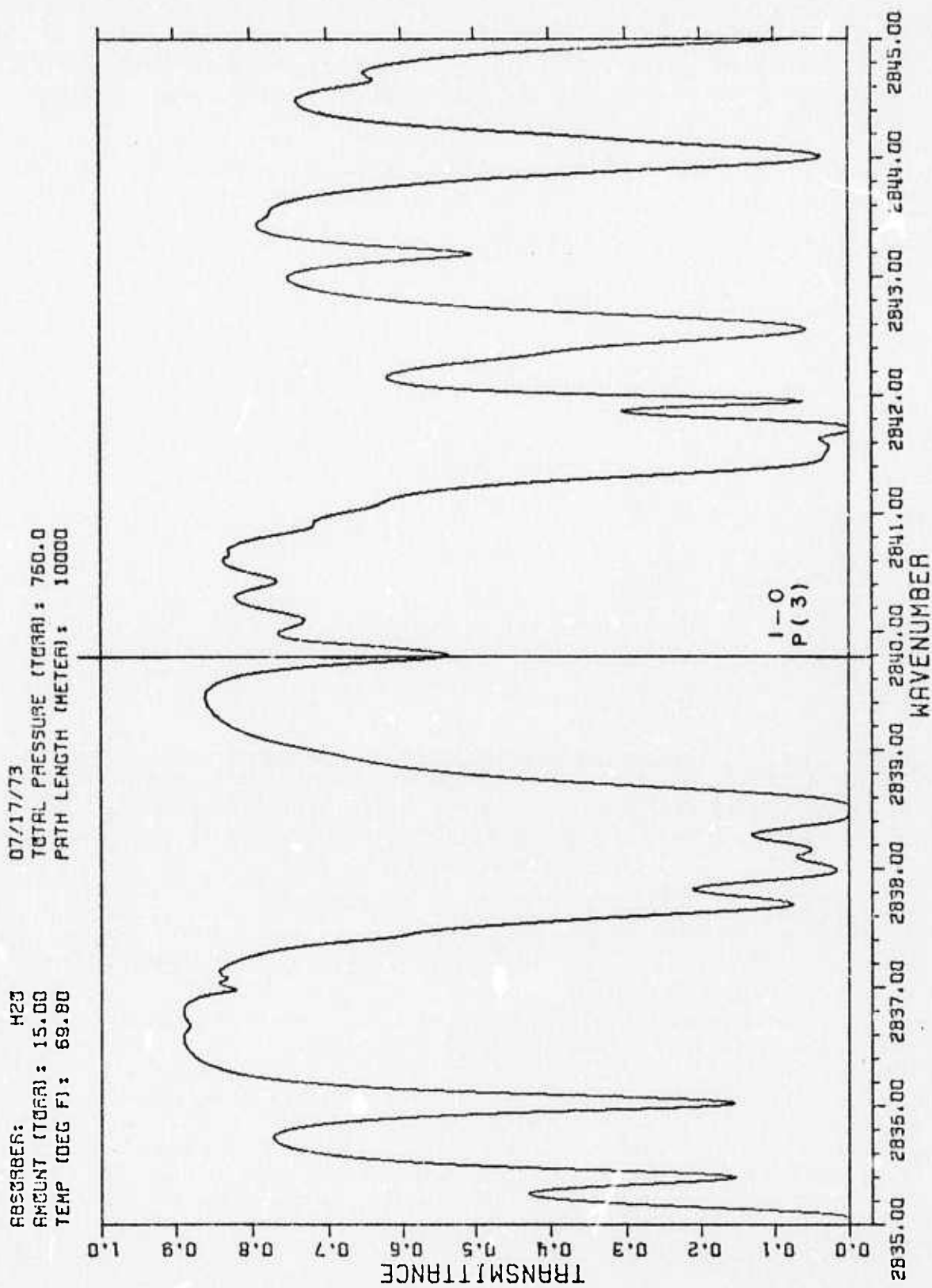


Fig. 54

SLOW was set to include all lines on the tape. DF line frequencies were for the purposes of the comparison set to the values in AFCRL-72-0312.

The results of the comparison are given in Table VI. The water

TABLE VI

LINE FREQUENCY (AFCRL)	LINE IDEN	$k_{\text{AFCRL}}$ (REPT. 72-0312)	$k_{\text{OSU}}$	$\frac{\Delta k}{\text{AFCRL}} \times 100$
2445.29	3-2,12	6.706E-2	7.007E-2	+ 4.5
2471.34	3-2,11	4.925E-2	5.598E-2	+13.7
2496.61	3-2,10	3.057E-2	2.966E-2	- 3.0
2500.32	2-1,13	2.445E-2	2.547E-2	+ 4.2
2521.81	3-2,9	1.521E-2	1.566E-2	+ 3.0
2527.47	2-1,12	1.419E-2	1.516E-2	+ 6.9
2546.37	3-2,8	3.262E-2	3.286E-2	+ 0.7
2553.97	2-1,11	1.462E-2	1.730E-2	+18.3
2570.51	3-2,7	5.098E-2	4.316E-2	-15.3
2580.16	2-1,10	2.808E-2	2.929E-2	+ 4.3
2594.23	3-2,6	9.654E-3	1.154E-2	+19.5
2605.87	2-1,9	2.337E-2	2.425E-2	+ 3.8
2611.10	1-0,12	8.700E-3	9.085E-3	+ 4.4
2617.41	3-2,5	4.165E-3	4.571E-3	+ 9.7
2631.09	2-1,8	7.276E-3	1.500E-2	+106.1
2655.97	2-1,7	4.094E-2	4.480E-2	+ 9.4
2665.20	1-0,10	1.861E-2	1.621E-2	-12.9
2680.28	2-1,6	4.569E-2	4.930E-2	+ 7.9
2703.98	2-1,5	4.132E-3	4.875E-2	+18.0
2727.38	2-1,4	2.663E-2	3.623E-2	+36.0
2750.05	2-1,3	3.023E-2	1.324E-2	-56.2

vapor continuum was not included in our computation since it was not included in AFCRL-72-0312[11].

Predictions made on the basis of the data tape and using a Lorentz line shape are not expected to be accurate to any better than 10 or 20 percent and in some cases at CO laser wavelengths we have experimental data[4] indicating that a much larger discrepancy exists. With respect to calculations made at two locations it is not clear why large discrepancies occur for some lines when the calculation and data input are supposedly identical.

In a calculation involving so much input data, it would probably take a significant joint effort to discover the reasons, and then it might simply be a legitimate difference in approach. At the present we do not have the funds to pursue the matter, if indeed it is worth pursuing, but we did feel that completeness required us to make the comparison, especially since we were using Dr. McClatchey's data and did not wish to make an obvious error in doing so.

The over one hundred percent difference for the 2-1 P(8) line bothers us since it is one of the high power DF lines, see Table IV.

Finally we should comment that the calculations were repeated using a super-Lorentz line shape[4] for water vapor but the results were nearly the same as for the Lorentz line shape. This is in opposition to the situation at  $5\mu$  where the water vapor coefficient was found to be very sensitive to line shape. Perhaps the reason is that here we do not have intense absorption lines so that the calculated coefficient is due to the lines near the calculation frequency. This could be tested by sharply lowering the value of BOUND to see if the effect on the absorption coefficient is small. This was not done, however.

Finally one notes that Table III includes predictions for nine 1-0 band DF frequencies which were not included in AFCRL-72-0312.



## APPENDIX A

We are indebted to Calfee[9] and McClatchey[5] for much of the material below.

### I. Conversion Factors

#### A. Conversion of (atm-cm)<sub>STP</sub> to molecules cm<sup>-2</sup>[5]

The molecular weight,  $M$ , of any gas in grams occupies 22.4136 liters at STP[12] so one cm<sup>3</sup> of any gas at STP weighs

$$\frac{M}{2.24136 \times 10^4} \text{ grams.}$$

Since 1 atm-cm<sub>STP</sub> is equivalent to one cm of gas at STP per cm<sup>2</sup>

$$1 \text{ atm-cm}_{\text{STP}} = \frac{M}{2.24136 \times 10^4} \text{ gm cm}^{-2}.$$

Avogadro's number[12] can be used to compute the number,  $n$ , of molecules per cm<sup>3</sup> of any gas

$$n = \frac{6.02252 \times 10^{23}}{2.24136 \times 10^4} = 2.687016 \times 10^{19} \text{ molecules cm}^{-3}.$$

Hence the desired result is

$$(1) \quad \boxed{\text{one atm-cm}_{\text{STP}} = 2.6870 \times 10^{19} \text{ molecules cm}^{-2}}.$$

#### B. Conversion of precipitable centimeters of water to mol cm<sup>-2</sup>[5]

$$1 \text{ atm-cm}_{\text{STP}, \text{H}_2\text{O}} = \frac{M}{2.24136 \times 10^4} = \frac{18.016}{2.24136 \times 10^4}$$

$$1 \text{ atm-cm}_{\text{STP}, \text{H}_2\text{O}} = 8.03798 \times 10^{-4} \text{ gm cm}^{-2}.$$

Using the constant developed in paragraph A, above we have the desired result

$$(2) \quad 1 \text{ pr-cm} = 3.3429 \times 10^{22} \text{ mol cm}^{-2} .$$

C. Partial pressure of water vapor from density and temperature[13].

From the referenced tables we have the relation

$$\rho = \frac{10^3 a \delta p_a / 760}{1 + \alpha T} \text{ gm m}^{-3}$$

where  $a$  = weight of one cubic meter of dry air at  $0^\circ\text{C}$  and 760 torr = 1.29278 kg.

$\delta$  = density of aqueous vapor relative to dry air = .62168

$p_a$  = partial pressure  $\text{H}_2\text{O}$  in torr

$\alpha$  = coefficient of expansion of air for  $1^\circ\text{C}$  = .00366.

Rearranging we have the desired result

$$(3) \quad p_a = .9456 (1 + .00366 T) \rho \text{ torr}$$

where  $T$  = temperature in deg C

$\rho$  = water vapor density in  $\text{gm/m}^3$

D. Precipitable centimeters  $\text{H}_2\text{O}$  from partial pressure, temperature, and path length

$$w = \rho \ell .$$

Using the relation from paragraph C,

$$w = \frac{1.05821 p_a \cdot 10^{-6}}{1 + .00367 (T_{\text{OK}} - 273.13)} \cdot \ell \cdot 10^2$$

where  $\ell$  is the path length in meters

$p_a$  is water vapor pressure in torr.

Since the third term in the denominator is nearly unity, we can write

$$(4) \quad w = \frac{2.8834 \times 10^{-2} p_a \ell}{T} \text{ pr-cm} .$$

E. Conversion to atm-cm<sub>STP</sub> from pressure, path length, and temperature of sample [5]

$$\text{atm-cm}_{\text{STP}} = \frac{\ell p_a}{760} \frac{273.13}{T}$$

$$(5) \quad \text{atm-cm}_{\text{STP}} = 3.5938 \times 10^{-1} \frac{p_a \ell}{T}$$

where  $p_a$  = absorber pressure in torr  
 $\ell$  = path length in cm  
 $T$  = temperature in deg K.

F. Density computed from partial pressure, molecular weight, and temperature

This is of course the Gas Law

$$(6) \quad \rho = 1.6035 \times 10^{-5} \frac{p_a M}{T} \text{ gm cm}^{-3}$$

where  $p_a$  = pressure in torr  
 $M$  = molecular weight  
 $T$  = deg K.

G. Partial pressure of water vapor from mixing ratio [14]

$$(7) \quad p_a = \frac{r P}{.62168 + r} \text{ torr}$$

where  $r$  is the mixing ratio and  $P$  is the total pressure in torr.

From the data in the AFCRL models (5), one should compute mixing ratio as follows:

$$(8) \quad r = \frac{p_{H_2O}}{p_{air} - p_{H_2O} \frac{28.9785}{18.0153}}$$

Note that the constant .62168 in Eq. (7) is the ratio of the molecular weight of water vapor to that of dry air at STP, i.e.,  $18.0153/28.9785$ , see reference 12. In the Smithsonian tables (14) the value used is 0.62197 apparently based on older molecular weight data.

H. Ozone partial pressure from density for AFCRL mid-latitude summer model (5)

$$(9) \quad p_a = \frac{d}{q} \times 760 \times \frac{6.0 \times 10^{-5}}{1.191 \times 10^3} \text{ torr}$$

where  $d$  = air density at STP = 28.9785 (12),  
 $q$  = molecular weight of ozone = 47.9982 (12),

and  $6.0 \times 10^{-5} \text{ g/m}^3$  is the density of ozone and  $1.191 \times 10^3 \text{ g/m}^3$  is the air density, both at sea level, of the AFCRL mid-latitude summer model. The result is  $2.31 \times 10^{-5} \text{ torr}$ .

# REFERENCES

1. McClatchey, R.A., et. al., AFCRL-TR-73-0096, January 1973.
2. McClatchey, R.A. and Selby, J.E.A., AFCRL-72-0312, May 1972.
3. Burch, D.E., Ford Aeronutronic Report U-4784, January 1970.
4. Long, R.K., Mills, F.S. and Trusty, G.L., "Experimental Absorption Coefficients for Eleven CO Laser Lines," Report 3271-5, March 1973, The Ohio State University ElectroScience Laboratory, Department of Electrical Engineering; prepared under Contract F30602-72-C-0016 for Rome Air Development Center. (RADC-TR-75-126) (AD 760 140).
5. McClatchey, R.A., et. al., AFCRL-72-0497, August 1972.
6. Rao, K.N., J. Mol. Spec., Vol. 16, p. 100, 1965.
7. Deutsch, T.F., Appl. Phys. Letters, Vol. 10, p. 234, 1967.
8. Burch, D.E., et. al., "Infrared Absorption by Minor Atmospheric Constituents," Ohio State University Research Foundation, Final Report, prepared under Contract AF 19(604)-2633, December 1960; also AFCRL 12.
9. Deutschman, E. M. and Calfee, R.F., "Two Computer Programs to Produce Theoretical Absorption Spectra of Water Vapor and Carbon Dioxide," AD 816 369, April 1967.
10. Calfee, R.F., "A Note on Terminologies Used in Gaseous Absorption Processes," NOAA Tech. Report ERL211-WPL-15, August 1971.
11. McClatchey, R.A., Private communication.
12. Handbook of Chemistry and Physics, 48th Edition, pp. F-158 and F-210, A-10, and rear coverpiece.
13. Smithsonian Meteorological Tables, Smithsonian Institute, 1951.
14. List, R.J., "Smithsonian Meteorological Tables," Sixth Revised Edition, p. 347, 1949.